

Two-grid methods for a class of nonlinear elliptic eigenvalue problems

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In this paper, we introduce and analyze some two-grid methods for nonlinear elliptic eigenvalue problems of the form $-\operatorname{div}(A\nabla u) + Vu + f(u^2)u = \lambda u$, $\|u\|_{L^2} = 1$. We provide *a priori* error estimates for the ground state energy, the eigenvalue λ , and the eigenfunction u , in various Sobolev norms. We focus in particular on the Fourier spectral approximation (for periodic boundary conditions), and on the \mathbb{P}_1 and \mathbb{P}_2 finite element discretizations (for homogeneous Dirichlet boundary conditions), taking numerical integration errors into account. Finally, we provide numerical examples illustrating our analysis.

Keywords: Nonlinear eigenvalue problem, Spectral and pseudo spectral approximation, Finite element approximation, Ground state computation, Numerical analysis, Two-grid method.

1. Introduction

Nonlinear eigenvalue problems are encountered in various applications in sciences and engineering, including the simulation of Bose-Einstein condensates (Gross-Pitaevskii equation, see e.g. Pitaevskii & Stringari (2003)), electronic structure calculation (Hartree-Fock method, orbital free and Kohn-Sham Density Functional Theory), and the study of the vibration modes of structures in nonlinear elasticity.

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The first results on the numerical analysis of nonlinear eigenvalue problems have been published in Zhou (2004). These first results were improved by three of us in Canc`es *et al.* (2010), where optimal *a priori* error bounds for nonlinear elliptic eigenvalue problems were obtained for the first time. The techniques introduced in Canc`es *et al.* (2010), based on estimates in negative Sobolev norms, have then been applied to a variety of nonlinear eigenvalue problems (see Canc`es *et al.* (2012); Chen *et al.* (2013)), among which the Kohn-Sham problem (Kohn & Sham (1965)), which is currently one of the most widely used models in computational physics and chemistry.

As in Canc`es *et al.* (2010), we focus on the nonlinear elliptic eigenvalue problems arising in the study of variational problems of the form

$$I = \inf \left\{ E(v), v \in X, \int_{\Omega} v^2 = 1 \right\}, \quad (1.1)$$

where

$$\left| \begin{array}{l} \Omega \text{ is a regular bounded domain or a rectangular brick of } \mathbb{R}^d \text{ and } X = H_0^1(\Omega), \\ \text{or} \\ \Omega \text{ is the unit cell of a periodic lattice } \mathcal{R} \text{ of } \mathbb{R}^d \text{ and } X = H_{\#}^1(\Omega), \end{array} \right.$$

with $d = 1, 2$, or 3 , $H_{\#}^1(\Omega)$ denoting the space of the restrictions to Ω of the H_{loc}^1 , \mathcal{R} -periodic functions on \mathbb{R}^d , and where the energy functional E is of the form

$$E(v) = \frac{1}{2}a(v, v) + \frac{1}{2} \int_{\Omega} F(v^2(x)) dx,$$

with

$$a(u, v) = \int_{\Omega} (A \nabla u) \cdot \nabla v + \int_{\Omega} V u v.$$

In all what follows, we assume that

- $A \in (L^{\infty}(\Omega))^{d \times d}$; $A(x)$ is symmetric for almost all $x \in \Omega$;
 $\exists \alpha > 0$ such that $\xi^T A(x) \xi \geq \alpha |\xi|^2$, $\forall \xi \in \mathbb{R}^d$ and almost all $x \in \Omega$; (1.2)

- $V \in L^p(\Omega)$ for some $p > \max(1, d/2)$; (1.3)

- $F \in C^1([0, +\infty), \mathbb{R}) \cap C^2((0, \infty), \mathbb{R})$, $F'(0) = 0$ and $F'' > 0$ on $(0, +\infty)$; (1.4)

- $\exists 0 \leq q < 2$, $\exists C \in \mathbb{R}_+$ such that $\forall t \geq 0$, $|F'(t)| \leq C(1 + t^q)$; (1.5)

- $F''(t)t$ is locally bounded on $[0, +\infty)$. (1.6)

To simplify the notation, we denote by f the derivative of F . Note that there is no loss of generality in assuming in (1.4) that $f(0) = F'(0) = 0$ since the minimizers of (1.1) are not modified if $F(t)$ is replaced with $F(t) + ct$.

Problem (1.1) has exactly two minimizers u and $-u$, one of them, say u , being positive on Ω . In all what follows, u will be the positive minimizer of (1.1). The function u is solution to the Euler-Lagrange equation

$$\forall v \in X, \quad \langle E'(u) - \lambda u, v \rangle_{X', X} = 0, \quad (1.7)$$

for some $\lambda \in \mathbb{R}$ (the Lagrange multiplier associated with the constraint $\|u\|_{L^2} = 1$) and equation (1.7), complemented with the constraint $\|u\|_{L^2} = 1$, takes the form of the nonlinear eigenvalue problem

$$\begin{cases} A_u u = \lambda u, \\ \|u\|_{L^2} = 1, \end{cases} \quad (1.8)$$

where for all $v \in X$,

$$A_v = -\operatorname{div}(A\nabla \cdot) + V + f(v^2)$$

is a linear self-adjoint operator on $L^2(\Omega)$ with form domain X . Note that $E'(u) = A_u u$. It can then be inferred from (1.8) that $u \in X \cap C^0(\overline{\Omega})$, $u > 0$ in Ω , and λ is the ground state eigenvalue of A_u . An important point is that λ is a *simple* eigenvalue of A_u . These results are classical; their proofs are recalled in Cancès *et al.* (2010).

We now consider a family of finite-dimensional subspaces $(X_\delta)_{\delta>0}$ of X such that

$$\forall v \in X, \quad \lim_{\delta \rightarrow 0} \min_{v_\delta \in X_\delta} \|v - v_\delta\|_{H^1} = 0 \quad (1.9)$$

and the variational approximations of (1.1) consisting in solving

$$I_\delta = \inf \left\{ E(v_\delta), v_\delta \in X_\delta, \int_\Omega v_\delta^2 = 1 \right\}. \quad (1.10)$$

Problem (1.10) has at least one minimizer u_δ such that $(u, u_\delta)_{L^2} \geq 0$, which satisfies

$$\forall v_\delta \in X_\delta, \quad \langle A_{u_\delta} u_\delta, v_\delta \rangle_{X', X} = \lambda_\delta (u_\delta, v_\delta)_{L^2},$$

for some $\lambda_\delta \in \mathbb{R}$. It is easily seen that (see, e.g., Cancès *et al.* (2010); Zhou (2004))

$$\lim_{\delta \rightarrow 0} \|u_\delta - u\|_{H^1} = 0, \quad (1.11)$$

or, in words, that the approximate ground state eigenfunction converges to the exact ground state eigenfunction in the H^1 -norm, from which we deduce that I_δ and λ_δ converge to I and λ , respectively, when δ goes to 0. Optimal convergence rates have been obtained in Cancès *et al.* (2010) (under stronger assumptions on the nonlinearity F) for finite element and spectral Fourier discretizations.

The numerical simulation of problem (1.10) can be too costly if the approximation space X_δ is high-dimensional. We will denote by X_{δ_f} such a space and call it the *fine discretization space*. In two-grid methods, problem (1.10) is first solved in a lower-dimensional approximation space $X_{\delta_c} \subset X_{\delta_f}$, that we will call the *coarse discretization space*. Then, the so-obtained solution u_{δ_c} is improved by solving a *linearized* problem in the fine discretization space X_{δ_f} . A nice feature of this approach is that, for appropriate choices of the linearized problem and of the coarse discretization space X_{δ_c} , the solution $u_{\delta_c}^{\delta_f}$ obtained with the two-grid method has the same accuracy as the solution u_{δ_f} obtained by solving the nonlinear problem (1.10) in the fine discretization space X_{δ_f} . Two-grid methods thus allow us to obtain the same accuracy at a much lower price. Such methods were first introduced in Xu & Zhou (2000) in the framework of nonlinear elliptic *boundary value* problems. A different two-grid approach is presented in Henning *et al.* (2013). The evaluation of its computational cost for a given accuracy with respect to our approach needs to be further analyzed.

This article is organized as follows. In Section 2, we introduce three different two-grid algorithms to solve (1.1). In Section 3, we provide some abstract *a priori* error analysis for one of these algorithms. We then show how these abstract results can be applied to spectral Fourier and finite element discretizations in Sections 4 and 5 respectively. Numerical integration errors are dealt with in Section 6. Finally, we give several numerical examples to illustrate our theoretical results in Section 7. The class of nonlinear eigenvalue problems considered in this work is very similar to the one considered in the previous

work Cancès *et al.* (2010) (only some assumptions on the nonlinearity F will differ). For this reason, some of the proofs of the results below are simple adaptations of proofs in Cancès *et al.* (2010), and will therefore not be detailed for the sake of brevity. Let us mention that some of the results contained in this article have been published (in French) in the PhD thesis of the second author (Chakir (2009)).

2. Two-grid algorithms

Let X_{δ_c} and X_{δ_f} be coarse and fine discretization spaces such that $X_{\delta_c} \subset X_{\delta_f} \subset X$. As mentioned above, two-grid methods consist, first in computing a solution of (1.10) in a coarse discretization space X_{δ_c} and, second in improving it by solving a linearized problem in the fine discretization space X_{δ_f} .

Several two-grid algorithms can therefore be proposed, depending on the type of linear problem we choose to solve in the fine discretization space. In the following, we introduce three of them, the first and third steps of these three schemes being the same.

1. Solve (1.10) in the *coarse* discretization space X_{δ_c} . Recall that the solution u_{δ_c} of this problem is such that there exists $\lambda_{\delta_c} \in \mathbb{R}$ such that $(\lambda_{\delta_c}, u_{\delta_c})$ is also solution to the *nonlinear* eigenvalue problem:

$$\begin{cases} \text{find } (\lambda_{\delta_c}, u_{\delta_c}) \in \mathbb{R} \times X_{\delta_c} \text{ such that} \\ \forall v_{\delta_c} \in X_{\delta_c}, \quad \langle A_{u_{\delta_c}} u_{\delta_c}, v_{\delta_c} \rangle_{X', X} = \lambda_{\delta_c} (u_{\delta_c}, v_{\delta_c})_{L^2}. \end{cases}$$

2. **Two-grid scheme 1.** Solve the following *linear eigenvalue* problem in the *fine* space X_{δ_f} :

$$\begin{cases} \text{find } (\lambda_{\delta_f}^{\delta_c}, u_{\delta_f}^{\delta_c}) \in \mathbb{R} \times X_{\delta_f} \text{ such that} \\ \forall v_{\delta_f} \in X_{\delta_f}, \quad a(u_{\delta_f}^{\delta_c}, v_{\delta_f}) + \int_{\Omega} f(u_{\delta_c}^2) u_{\delta_f}^{\delta_c} v_{\delta_f} = \lambda_{\delta_f}^{\delta_c} \int_{\Omega} u_{\delta_f}^{\delta_c} v_{\delta_f}, \\ \|u_{\delta_f}^{\delta_c}\|_{L^2} = 1, \quad (u, u_{\delta_f}^{\delta_c})_{L^2} \geq 0, \\ \lambda_{\delta_f}^{\delta_c} \text{ is the lowest eigenvalue of the above spectral problem.} \end{cases} \quad (2.1)$$

Two-grid scheme 2a. Solve the following *linearized right-hand side* problem in the *fine* space X_{δ_f} :

$$\begin{cases} \text{find } u_{\delta_f}^{\delta_c} \in X_{\delta_f} \text{ such that} \\ \forall v_{\delta_f} \in X_{\delta_f}, \quad a(u_{\delta_f}^{\delta_c}, v_{\delta_f}) + \int_{\Omega} f(u_{\delta_c}^2) u_{\delta_f}^{\delta_c} v_{\delta_f} = \lambda_{\delta_c} \int_{\Omega} u_{\delta_c} v_{\delta_f}. \end{cases}$$

Two-grid scheme 2b. Solve the following *linearized right-hand side* problem in the *fine* space X_{δ_f} :

$$\begin{cases} \text{find } u_{\delta_f}^{\delta_c} \in X_{\delta_f} \text{ such that} \\ \forall v_{\delta_f} \in X_{\delta_f}, \quad a(u_{\delta_f}^{\delta_c}, v_{\delta_f}) = - \int_{\Omega} f(u_{\delta_c}^2) u_{\delta_c} v_{\delta_f} + \lambda_{\delta_c} \int_{\Omega} u_{\delta_c} v_{\delta_f}. \end{cases}$$

3. Compute the Rayleigh quotient $\tilde{\lambda}_{\delta_f}^{\delta_c}$ for $u_{\delta_f}^{\delta_c}$:

$$\tilde{\lambda}_{\delta_f}^{\delta_c} = \frac{\langle A_{u_{\delta_f}^{\delta_c}} u_{\delta_f}^{\delta_c}, u_{\delta_f}^{\delta_c} \rangle_{X', X}}{\|u_{\delta_f}^{\delta_c}\|_{L^2}^2}. \quad (2.2)$$

In the limit $\delta_f = 0$ (that corresponds to $X_{\delta_f} = X$), the second step of scheme 1 amounts to computing the ground state $(\lambda_0^{\delta_c}, u_0^{\delta_c})$ of the self-adjoint operator $A_{u_{\delta_c}}$, while schemes 2a and 2b amount to solving the boundary value problems $A_{u_{\delta_c}} u_0^{\delta_c} = \lambda_{\delta_c} u_{\delta_c}$ and $A_0 u_0^{\delta_c} = (\lambda_{\delta_c} - f(u_{\delta_c}^2)) u_{\delta_c}$, respectively.

In this paper, we shall focus on the analysis of the first scheme, both from the theoretical and simulation points of view. The analysis of the other two schemes will be the matter of a forthcoming work. Let us just mention here that on preliminary simulations, schemes 2a and 2b provide similar results as scheme 1 (see Chakir (2009)).

3. Abstract error analysis of scheme 1

We denote by u the unique positive solution of (1.1), by u_{δ_c} a minimizer of the discretized nonlinear problem (1.10) such that $(u, u_{\delta_c})_{L^2} \geq 0$, and by $u_{\delta_f}^{\delta_c}$ the approximation of u computed with scheme 1. The aim of this section is to establish error bounds on $\|u - u_{\delta_f}^{\delta_c}\|_{H^1}$, $\|u - u_{\delta_f}^{\delta_c}\|_{L^2}$ and $|\lambda - \lambda_{\delta_f}^{\delta_c}|$, in the general framework of assumptions (1.2)-(1.6) and (1.9).

3.1 Preliminaries

Our analysis relies on the introduction of the solution $u_0^{\delta_c}$ of the two-grid scheme in the limiting case when $\delta_f = 0$ (that is for $X_{\delta_f} = X$). Recall that $u_0^{\delta_c}$ is the positive ground state eigenfunction of $A_{u_{\delta_c}}$. We denote by $\lambda_0^{\delta_c}$ the associated eigenvalue. The minmax principle gives

$$\lambda_0^{\delta_c} = \inf \left\{ \langle A_{u_{\delta_c}} v, v \rangle_{X', X}, v \in X, \int_{\Omega} v^2 = 1 \right\}, \quad (3.1)$$

and the solution $(\lambda_{\delta_f}^{\delta_c}, u_{\delta_f}^{\delta_c})$ provided by the two-grid scheme 1 can then be interpreted as the solution of the variational approximation

$$\lambda_{\delta_f}^{\delta_c} = \inf \left\{ \langle A_{u_{\delta_c}} v_{\delta_f}, v_{\delta_f} \rangle_{X', X}, v_{\delta_f} \in X_{\delta_f}, \int_{\Omega} v_{\delta_f}^2 = 1 \right\} \quad (3.2)$$

of problem (3.1) in the discretization space X_{δ_f} .

Problem (3.2) has at least one minimizer $u_{\delta_f}^{\delta_c}$, which satisfies (2.1), for some $\lambda_{\delta_f}^{\delta_c} \in \mathbb{R}$. Note that, when $\delta_f = \delta_c$, $u_{\delta_c}^{\delta_c} = u_{\delta_c}$ is solution to (3.2).

The following numerical analysis relies on the properties of the mapping $v \mapsto (\lambda_v, z_v)$, where λ_v denotes the lowest eigenvalue of the self-adjoint operator A_v and $z_v > 0$ the associated positive normalized eigenfunction:

$$\begin{cases} A_v z_v = \lambda_v z_v, \\ z_v > 0, \\ \|z_v\|_{L^2} = 1. \end{cases}$$

The function z_v is also the minimizer of the problem

$$\inf \left\{ \langle A_v w, w \rangle_{X', X}, w \in X, \int_{\Omega} w^2 = 1 \right\},$$

(which amounts to minimizing the Rayleigh quotient associated with the self-adjoint operator A_v). In the special case when $v = u$, we have $(\lambda_u, z_u) = (\lambda, u)$.

The following technical lemmas will be used throughout the article. For the reader's convenience, we first state all the lemmas, and postpone their proofs until the end of the section.

LEMMA 3.1 Under assumptions (1.2), there exist $\beta_0 \in \mathbb{R}_+$ and $M \in \mathbb{R}_+$ such that

$$\forall w \in X, \quad \frac{\alpha}{2} \|\nabla w\|_{L^2}^2 - \beta_0 \|w\|_{L^2}^2 \leq a(w, w) \leq M \|w\|_{H^1}^2. \quad (3.3)$$

We recall that f denotes the derivative of F and u the unique positive minimizer of (1.1) that satisfies $A_u u = \lambda u$ with $\lambda \in \mathbb{R}$.

LEMMA 3.2 Assume that F satisfies assumptions (1.4)-(1.6). Denoting by $r = \frac{6}{5-2q}$ ($\frac{6}{5} \leq r < 6$), there exists a constant $C \in \mathbb{R}_+$ such that for all $(v, w, z) \in X^3$,

$$\left| \int_{\Omega} f(v^2) wz \right| \leq C \left(1 + \|v\|_{L^6}^{2q} \right) \|w\|_{L^6} \|z\|_{L^r}, \quad (3.4)$$

$$\left| \int_{\Omega} (f(v^2) - f(u^2)) uw \right| \leq C \left(1 + \|v\|_{L^6}^{2q} \right) \|w\|_{L^6} \|u - v\|_{L^r}, \quad (3.5)$$

$$\left| \int_{\Omega} (f(v^2) - f(u^2)) v^2 \right| \leq C \left(1 + \|v\|_{L^6}^{2q+1} \right) \|u - v\|_{L^r}, \quad (3.6)$$

$$0 \leq \int_{\Omega} F(v^2) - F(u^2) - f(u^2) (v^2 - u^2) \leq C \left(1 + \|v\|_{L^6}^{2q+1} \right) \|u - v\|_{L^r}. \quad (3.7)$$

Besides, in the case where $X = H_{\#}^1(\Omega)$, there exists $C \in \mathbb{R}_+$ such that for all $(v, w) \in X^2$,

$$\int_{\Omega} (f(u^2) - f(v^2)) w^2 \leq C \int_{\Omega} \mathbb{1}_{u \geq |v|} (u - v) w^2 \quad (X = H_{\#}^1(\Omega) \text{ only}), \quad (3.8)$$

while, in the case where $X = H_0^1(\Omega)$, for all $\varepsilon > 0$, there exists $C_{\varepsilon} \in \mathbb{R}_+$ such that for all $(v, w) \in X^2$,

$$\int_{\Omega} (f(u^2) - f(v^2)) w^2 \leq \varepsilon \|w\|_{L^2}^2 + C_{\varepsilon} \int_{\Omega} \mathbb{1}_{u \geq |v|} (u - v) w^2 \quad (X = H_0^1(\Omega) \text{ only}). \quad (3.9)$$

LEMMA 3.3 There exist $0 < M_2 \leq M_1 < \infty$ such that

$$\forall v \in X, \quad 0 \leq \langle (A_u - \lambda)v, v \rangle_{X', X} \leq M_1 \|v\|_{H^1}^2, \quad (3.10)$$

and

$$\forall v \in u^{\perp} := \{v \in X, (u, v)_{L^2} = 0\}, \quad M_2 \|v\|_{H^1}^2 \leq \langle (A_u - \lambda)v, v \rangle_{X', X}. \quad (3.11)$$

Moreover, there exists $\gamma > 0$ such that, for all $w \in X$ such that $\|w\|_{L^2} = 1$ and $(u, w)_{L^2} \geq 0$,

$$\gamma \|w - u\|_{H^1}^2 \leq \langle (A_u - \lambda)(w - u), (w - u) \rangle_{X', X}. \quad (3.12)$$

The properties of the ground state eigenpair (λ_v, z_v) of A_v are collected in the following lemma.

LEMMA 3.4 There exists a constant $C \in \mathbb{R}_+$ such that

$$\forall v \in X, \quad |\lambda_v| + \|z_v\|_{H^1}^2 \leq C \left(1 + \|v\|_{L^6}^{2q} \right), \quad (3.13)$$

$$\forall v \in X, \quad \|z_v - u\|_{H^1} \leq C \left(1 + \|v\|_{L^6}^{2q} \right) \|u - v\|_{L^{\max(r, 2)}}. \quad (3.14)$$

In addition,

- in the case when $X = H_{\#}^1(\Omega)$, there exists $C \in \mathbb{R}_+$ such that

$$\forall v \in X, \quad |\lambda_v - \lambda| \leq C \left(1 + \|v\|_{L^6}^{2q}\right) \|v - u\|_{L^{\max(r,2)}} \quad (X = H_{\#}^1(\Omega) \text{ only}); \quad (3.15)$$

- in the case when $X = H_0^1(\Omega)$, there exists, for any $\varepsilon > 0$, a constant $C_{\varepsilon} \in \mathbb{R}_+$ such that

$$\forall v \in X, \quad |\lambda_v - \lambda_u| \leq 2\varepsilon + C_{\varepsilon} \left(1 + \|v\|_{L^6}^{2q}\right) \|u - v\|_{L^{\max(r,2)}} \quad (X = H_0^1(\Omega) \text{ only}). \quad (3.16)$$

Estimates (3.15)-(3.16) are sufficient for our purpose, but are not optimal; refined estimates are actually given in the proof of Lemma 3.4.

For all $v \in X$, we denote by $\lambda_{2,v}$ the second eigenvalue of A_v . Since $\lambda = \lambda_u$ is a simple eigenvalue of A_u , there is a gap, denoted by $g = \lambda_{2,u} - \lambda_u > 0$, between the first and second eigenvalues of A_u .

LEMMA 3.5 There exists $0 < \eta \leq 1$ such that for all $v \in X$ such that $\|v - u\|_{H^1} \leq \eta$, we have $\lambda_{2,v} - \lambda_v \geq g/2$.

PROPOSITION 3.1 There exist $\eta > 0$ and $0 < c_0 \leq C_0 < \infty$ such that for all $v \in X$ such that $\|v - u\|_{H^1} \leq \eta$ and all $w \in X$ such that $\|w\|_{L^2} = 1$ and $(z_v, w)_{L^2} \geq 0$, we have

$$c_0 \|w - z_v\|_{H^1}^2 \leq \langle (A_v - \lambda_v)(w - z_v), (w - z_v) \rangle_{X', X} \leq C_0 \|w - z_v\|_{H^1}^2. \quad (3.17)$$

Proof of Lemma 3.1. For brevity, we only explain in detail the arguments for $d = 3$, in which case $p > 3/2$. Under assumptions (1.2), there exists a positive constant M such that

$$\forall w \in X, \quad a(w, w) \leq \|A\|_{L^\infty} \|\nabla w\|_{L^2}^2 + \|V\|_{L^p} \|w\|_{L^{2p'}}^2 \leq M \|w\|_{H^1}^2,$$

where $1 \leq p' = (1 - p^{-1})^{-1} < 3$. Using Hölder's inequality, we have that for any $w \in X$,

$$\begin{aligned} a(w, w) &= \int_{\Omega} A \nabla w \cdot \nabla w + \int_{\Omega} V w^2 \\ &\geq \alpha \|\nabla w\|_{L^2}^2 - \|V\|_{L^p} \|w\|_{L^2}^{2-3/p} \|w\|_{L^6}^{3/p} \\ &\geq \alpha \|\nabla w\|_{L^2}^2 - C_6^{3/p} \|V\|_{L^p} \|w\|_{L^2}^{2-3/p} \|w\|_{H^1}^{3/p}, \end{aligned}$$

where C_6 is the Sobolev constant such that for all $v \in X$, $\|v\|_{L^6} \leq C_6 \|v\|_{H^1}$.

Using Young's inequality, we have for all $\varepsilon > 0$ and $w \in X$,

$$\begin{aligned} C_6^{3/p} \|V\|_{L^p} \|w\|_{L^2}^{2-3/p} \|w\|_{H^1}^{3/p} &= \left(\frac{1}{\varepsilon} C_6^{3/p} \|V\|_{L^p} \|w\|_{L^2}^{2-3/p} \right) (\varepsilon \|w\|_{H^1}^{3/p}) \\ &\leq \frac{2p-3}{2p} \left(\frac{1}{\varepsilon} C_6^{3/p} \|V\|_{L^p} \|w\|_{L^2}^{2-3/p} \right)^{2p/(2p-3)} + \frac{3}{2p} (\varepsilon \|w\|_{H^1}^{3/p})^{2p/3} \\ &= \frac{2p-3}{2p} \left(\left(\frac{1}{\varepsilon} C_6^{3/p} \|V\|_{L^p} \right)^{2p/3} \right)^{3/(2p-3)} \|w\|_{L^2}^2 + \frac{3}{2p} \varepsilon^{2p/3} \|w\|_{H^1}^2. \end{aligned}$$

Choosing $\frac{3}{2p} \varepsilon^{2p/3} = \frac{\alpha}{2}$, we get

$$C_6^{3/p} \|V\|_{L^p} \|w\|_{L^2}^{2-3/p} \|w\|_{H^1}^{3/p} \leq \frac{2p-3}{2p} \left(\frac{3}{p\alpha} C_6^{3/p} \|V\|_{L^p}^{2p/3} \right)^{3/(2p-3)} \|w\|_{L^2}^2 + \frac{\alpha}{2} \|w\|_{L^2}^2 + \frac{\alpha}{2} \|\nabla w\|_{L^2}^2,$$

which implies

$$a(w, w) \geq \frac{\alpha}{2} \|\nabla w\|_{L^2}^2 - \left(\frac{2p-3}{2p} \left(\frac{3}{p\alpha} C_6^2 \|v\|_{L^p}^{2p/3} \right)^{3/(2p-3)} + \frac{\alpha}{2} \right) \|w\|_{L^2}^2.$$

Hence, there exists a positive constant β_0 such that

$$\forall w \in X, \quad a(w, w) \geq \frac{\alpha}{2} \|\nabla w\|_{L^2}^2 - \beta_0 \|w\|_{L^2}^2.$$

This completes the proof. \square

Proof of Lemma 3.2. In this proof, C denotes a non-negative constant independent on v , w and z , but whose value is allowed to change from one line to another. We recall that $r = \frac{6}{5-2q}$.

Proof of (3.4). It follows from assumption (1.5) that for all $(v, w, z) \in X$,

$$\left| \int_{\Omega} f(v^2) wz \right| \leq C \int_{\Omega} (1 + |v|^{2q}) |w| |z| \leq C \left(1 + \|v\|_{L^6}^{2q} \right) \|w\|_{L^6} \|z\|_{L^r}.$$

Proof of (3.5). We first write

$$\int_{\Omega} (f(v^2) - f(u^2)) u w = \int_{\Omega} \tilde{w}_{v,u} (u - v) w, \quad \text{with} \quad \tilde{w}_{v,u} = -\frac{f(u^2) - f(v^2)}{u - v} u. \quad (3.18)$$

Since $u \in L^\infty(\Omega)$ and $u \geq 0$, it holds

$$|\tilde{w}_{v,u}| \leq \begin{cases} 2(f(v^2) + f(\|u\|_{L^\infty}^2)), & \text{when } |v| < u/2, \\ 4 \sup_{t \in (0, 4\|u\|_{L^\infty}^2]} F''(t) t, & \text{when } u/2 \leq |v| < 2u, \\ |f(v^2)| + f(\|u\|_{L^\infty}^2), & \text{when } |v| \geq 2u. \end{cases} \quad (3.19)$$

The above estimate is easily obtained in the case when $|v| < u/2$ or $|v| \geq 2u$. When $u/2 \leq |v| < 2u$, we observe that

$$|f(u^2) - f(v^2)| = \left| \int_{u^2}^{v^2} F''(t) dt \right| = \left| \int_{u^2}^{v^2} \frac{t F''(t)}{t} dt \right| \leq 2 \left(\sup_{t \in (0, 4\|u\|_{L^\infty}^2]} F''(t) t \right) |\ln u - \ln |v||.$$

It follows that when $u/2 \leq |v| < 2u$, there exists $u/2 \leq \xi < 2u$ such that

$$|\tilde{w}_{v,u}| \leq 2 \left(\sup_{t \in (0, 4\|u\|_{L^\infty}^2]} F''(t) t \right) \left| \frac{\ln u - \ln |v|}{u - v} \right| u = 2 \left(\sup_{t \in (0, 4\|u\|_{L^\infty}^2]} F''(t) t \right) \frac{u}{\xi} \leq 4 \sup_{t \in (0, 4\|u\|_{L^\infty}^2]} F''(t) t.$$

Thus, (3.19) is proved. This estimate, together with assumptions (1.5) and (1.6), yields

$$|\tilde{w}_{v,u}| \leq C (1 + |v|^{2q}),$$

which, combined with (3.18), straightforwardly leads to (3.5).

Proof of (3.6). For all $v \in X$, we can write

$$\int_{\Omega} (f(v^2) - f(u^2)) v^2 = \int_{\Omega} w_{v,u} (v - u), \quad \text{with} \quad w_{v,u} = v^2 \frac{f(v^2) - f(u^2)}{v - u}. \quad (3.20)$$

As $u \in L^\infty(\Omega)$, we have (see the proof of (Cancès *et al.*, 2010, Theorem 1))

$$|w_{v,u}| \leq \begin{cases} 12u \sup_{t \in (0, 4\|u\|_{L^\infty}^2]} F''(t)t, & \text{when } |v| < 2u, \\ 2(|f(v^2)| + f(\|u\|_{L^\infty}^2))|v|, & \text{when } |v| \geq 2u. \end{cases}$$

We infer from assumptions (1.5) and (1.6) that

$$|w_{v,u}| \leq C(1 + |v|^{2q+1}). \quad (3.21)$$

Putting together (3.20) and (3.21), we obtain

$$\left| \int_{\Omega} (f(v^2) - f(u^2))v^2 \right| \leq \|w_{v,u}\|_{L^{6/(1+2q)}} \|u - v\|_{L^r} \leq C \left(1 + \|v\|_{L^6}^{2q+1}\right) \|u - v\|_{L^r}.$$

Proof of (3.7). The left-hand side inequality in (3.7) follows from the convexity of F (assumption (1.4)). On the other hand,

$$\forall v \in X, \quad \int_{\Omega} F(v^2) - F(u^2) - f(u^2)(v^2 - u^2) = \int_{\Omega} (f(\xi) - f(u^2))(v^2 - u^2)$$

with $\xi \in [\min(u^2, v^2), \max(u^2, v^2)]$. Using assumption (1.5) and the boundedness of u , we get

$$\int_{\Omega} F(v^2) - F(u^2) - f(u^2)(v^2 - u^2) \leq C \int_{\Omega} (1 + |v|^{2q+1}) |u - v| \leq C \left(1 + \|v\|_{L^6}^{2q+1}\right) \|u - v\|_{L^r}.$$

Proof of (3.8). We assume here that $X = H_{\#}^1(\Omega)$. Since u is continuous, everywhere positive, and periodic, there exists a positive constant α_0 such that $u \geq \alpha_0 > 0$.

Denoting by $\Omega_- = \{x \in \Omega \mid |v(x)| < \frac{\alpha_0}{2}\}$ and $\Omega_+ = \{x \in \Omega \mid |v(x)| \geq \frac{\alpha_0}{2}\}$, we have

$$\forall (v, w) \in X^2, \quad \int_{\Omega} (f(u^2) - f(v^2))w^2 = \int_{\Omega_-} (f(u^2) - f(v^2))w^2 + \int_{\Omega_+} (f(u^2) - f(v^2))w^2. \quad (3.22)$$

Since, over Ω_- , v is such that $|v| < u \leq \|u\|_{L^\infty}$ and f is monotonically increasing, we have $|f(v^2)| \leq |f(\|u\|_{L^\infty}^2)|$ over Ω_- , so that

$$\begin{aligned} \int_{\Omega_-} (f(u^2) - f(v^2))w^2 &\leq 2f(\|u\|_{L^\infty}^2) \int_{\Omega_-} \frac{u - v}{u - v} w^2 \\ &\leq \frac{4f(\|u\|_{L^\infty}^2)}{\alpha_0} \int_{\Omega_-} (u - v)w^2 \\ &\leq C \int_{\Omega_-} (u - v)w^2. \end{aligned} \quad (3.23)$$

Denoting by $\Omega_+^1 = \{x \in \Omega \mid u(x) > |v(x)| \geq \frac{\alpha_0}{2}\}$ and $\Omega_+^2 = \{x \in \Omega \mid |v(x)| \geq u(x) \geq \alpha_0\}$, and using the fact that f is monotonically increasing, we obtain

$$\begin{aligned} \int_{\Omega_+} (f(u^2) - f(v^2))w^2 &= \int_{\Omega_+^1} (f(u^2) - f(v^2))w^2 + \int_{\Omega_+^2} (f(u^2) - f(v^2))w^2 \\ &\leq \int_{\Omega_+^1} (f(u^2) - f(v^2))w^2 \\ &= \int_{\Omega_+^1} f'(\xi)(u^2 - v^2)w^2, \end{aligned}$$

where $\xi \in [v^2, u^2] \subset [\alpha_0^2/4, \|u\|_{L^\infty}^2]$. Since $F \in C^2((0, \infty), \mathbb{R})$ (assumption (1.4)), we get

$$\int_{\Omega_+} (f(u^2) - f(v^2))w^2 \leq C \int_{\Omega_+^1} (u^2 - v^2)w^2 \leq C \int_{\Omega_+^1} 2u(u - v)w^2 \leq C \int_{\Omega_+^1} (u - v)w^2. \quad (3.24)$$

Combining (3.22), (3.23), and (3.24), we obtain (3.8).

Proof of (3.9). We now consider the case when $X = H_0^1(\Omega)$. Since $F \in C^1([0, +\infty), \mathbb{R})$ and $f(0) = 0$, there exists, for any $\varepsilon > 0$, a constant $\beta_\varepsilon > 0$ such that for all $0 \leq t \leq \beta_\varepsilon^2$,

$$|f(t)| \leq \varepsilon. \quad (3.25)$$

Since f is monotonically increasing, we have for all $(v, w) \in X^2$,

$$\begin{aligned} \int_{\Omega} (f(u^2) - f(v^2))w^2 &= \int_{\Omega} \mathbb{1}_{u \leq |v|} (f(u^2) - f(v^2))w^2 + \int_{\Omega} \mathbb{1}_{u > |v|} (f(u^2) - f(v^2))w^2 \\ &\leq \int_{\Omega} \mathbb{1}_{u > |v|} (f(u^2) - f(v^2))w^2. \end{aligned} \quad (3.26)$$

Denoting by $\Omega_{1,\varepsilon} = \{x \in \Omega \mid 0 \leq |v(x)| < u(x) < \beta_\varepsilon\}$, $\Omega_{2,\varepsilon} = \{x \in \Omega \mid 0 \leq |v(x)| < \beta_\varepsilon/2, u(x) \geq \beta_\varepsilon\}$, and $\Omega_{3,\varepsilon} = \{x \in \Omega \mid \beta_\varepsilon/2 < |v(x)| < u(x)\}$, we split the right-hand side of (3.26) into three parts. Using (3.25) and the boundedness of u , we get

$$\int_{\Omega_{1,\varepsilon}} (f(u^2) - f(v^2))w^2 \leq 2\varepsilon \|w\|_{L^2}^2,$$

and

$$\int_{\Omega_{2,\varepsilon}} (f(u^2) - f(v^2))w^2 \leq \frac{4}{\beta_\varepsilon} f(\|u\|_{L^\infty}^2) \int_{\Omega_{2,\varepsilon}} (u - v)w^2.$$

We then note that there exists ξ with $v^2 \leq \xi \leq u^2$ such that

$$\int_{\Omega_{3,\varepsilon}} (f(u^2) - f(v^2))w^2 = \int_{\Omega_{3,\varepsilon}} f'(\xi)(u^2 - v^2)w^2 \leq 2 \left(\max_{t \in [\beta_\varepsilon^2/4, \|u\|_{L^\infty}^2]} F''(t) \right) \|u\|_{L^\infty} \int_{\Omega_{3,\varepsilon}} (u - v)w^2.$$

Thus, (3.9) is proved with $C_\varepsilon = \frac{4}{\beta_\varepsilon} f(\|u\|_{L^\infty}^2) + 2 \left(\max_{t \in [\beta_\varepsilon^2/4, \|u\|_{L^\infty}^2]} F''(t) \right) \|u\|_{L^\infty}$. \square

Proof of Lemma 3.3. The detailed proof of (3.10) and (3.11) can be found in Cancès *et al.* (2010). Let us prove (3.12). We know from inequality (20) in Cancès *et al.* (2010) that there exists $\eta > 0$ such that

$$\forall v \in X, \quad \langle (A_u - \lambda)v, v \rangle_{X', X} \geq \eta (\|v\|_{L^2}^2 - |(u, v)_{L^2}|^2) \geq 0. \quad (3.27)$$

Since $\|w\|_{L^2} = 1$ and $\|u\|_{L^2} = 1$, we have

$$\|w - u\|_{L^2}^2 - |(w - u, u)_{L^2}|^2 \geq \|w - u\|_{L^2}^2 - (1 - (w, u)_{L^2})^2 = \frac{1}{2} \|w - u\|_{L^2}^2,$$

which together with (3.27) implies

$$\langle (A_u - \lambda)(w - u), (w - u) \rangle_{X', X} \geq \frac{\eta}{2} \|w - u\|_{L^2}^2. \quad (3.28)$$

In view of inequality (22) in Cancès *et al.* (2010), there exists a constant $C \in \mathbb{R}_+$ such that

$$\langle (A_u - \lambda)(w - u), (w - u) \rangle_{X', X} \geq \frac{\alpha}{2} \|\nabla(w - u)\|_{L^2}^2 - C \|w - u\|_{L^2}^2. \quad (3.29)$$

We obtain (3.12) with $\gamma = \frac{\alpha\eta}{2(\eta+2C)}$ by combining (3.28) and (3.29). \square

Proof of Lemma 3.4. In this proof, C , C_1 , C_2 denote non-negative constants independent of v , but whose values are allowed to change from one line to another. As λ_v is the lowest eigenvalue of A_v , we infer from (1.4), (3.3) and the boundedness of u that

$$\begin{aligned} \lambda_v &= \langle A_v z_v, z_v \rangle_{X', X} \leq \langle A_v u, u \rangle_{X', X} = a(u, u) + \int_{\Omega} f(v^2) u^2 \\ &\leq M \|u\|_{H^1}^2 + C \left(1 + \|v\|_{L^{2q}}^{2q}\right) \leq C \left(1 + \|v\|_{L^{2q}}^{2q}\right). \end{aligned} \quad (3.30)$$

Using (3.3), the fact that $\|z_v\|_{L^2} = 1$, and the positivity of $F''(t)$ (which implies that $f(t^2) \geq 0$ for all $t \in \mathbb{R}$), we obtain

$$\lambda_v = a(z_v, z_v) + \int_{\Omega} f(v^2) z_v^2 \geq \frac{\alpha}{2} \|z_v\|_{H^1}^2 - \frac{\alpha}{2} - \beta_0,$$

which, together with (3.30), readily leads to (3.13).

We now turn to the proof of (3.15) and (3.16). Let $v \in X$. We shall analyze each case of the alternative $\lambda_v > \lambda = \lambda_u$ or $\lambda_v \leq \lambda = \lambda_u$. In the former case, since λ_v is the lowest eigenvalue of A_v , we have

$$\lambda < \lambda_v = \langle A_v z_v, z_v \rangle_{X', X} \leq \langle A_v u, u \rangle_{X', X} = \lambda + \int_{\Omega} (f(v^2) - f(u^2)) u^2.$$

In the latter case, we use this time the fact that λ_u is the lowest eigenvalue of A_u to get

$$\lambda_v \leq \lambda = \langle A_u u, u \rangle_{X', X} \leq \langle A_u z_v, z_v \rangle_{X', X} = \lambda_v + \int_{\Omega} (f(u^2) - f(v^2)) z_v^2.$$

Therefore, using either (3.5) with $w = u$ (former case), or (3.8)-(3.9) with $w = z_v$ and (3.13) (latter case), we obtain that, for all $v \in X$,

$$|\lambda_v - \lambda| \leq C \left(1 + \|v\|_{L^6}^{2q}\right) \|u - v\|_{L^{\max(r, 2)}} \quad (X = H_{\#}^1(\Omega) \text{ only})$$

and

$$|\lambda_v - \lambda| \leq 2\varepsilon + C_{\varepsilon} \left(1 + \|v\|_{L^6}^{2q}\right) \|u - v\|_{L^{\max(r, 2)}} \quad (X = H_0^1(\Omega) \text{ only}).$$

Since $\lambda_v z_v - \lambda_u u = A_v z_v - A_u u$, we have

$$\begin{aligned} (\lambda_v z_v - \lambda_u u, z_v - u) &= \langle A_v z_v - A_u u, z_v - u \rangle_{X', X} \\ &= a(z_v - u, z_v - u) + \int_{\Omega} f(v^2) z_v (z_v - u) - \int_{\Omega} f(u^2) u (z_v - u) \\ &= a(z_v - u, z_v - u) + \int_{\Omega} f(u^2) (z_v - u)^2 + \int_{\Omega} (f(v^2) - f(u^2)) z_v (z_v - u) \\ &= \langle A_u (z_v - u), (z_v - u) \rangle_{X', X} + \int_{\Omega} (f(v^2) - f(u^2)) z_v (z_v - u). \end{aligned}$$

Hence, we have

$$\langle (A_u - \lambda_u)(z_v - u), (z_v - u) \rangle_{X', X} = (\lambda_v - \lambda_u) \int_{\Omega} z_v(z_v - u) + \int_{\Omega} (f(u^2) - f(v^2)) z_v(z_v - u),$$

which together with (3.12) implies that

$$\begin{aligned} \gamma \|z_v - u\|_{H^1}^2 &\leq (\lambda_v - \lambda_u) \int_{\Omega} z_v(z_v - u) + \int_{\Omega} (f(u^2) - f(v^2)) z_v(z_v - u) \\ &= \frac{1}{2} (\lambda_v - \lambda_u) \|z_v - u\|_{L^2}^2 + \int_{\Omega} (f(u^2) - f(v^2)) u(z_v - u) + \int_{\Omega} (f(u^2) - f(v^2)) (z_v - u)^2. \end{aligned}$$

To conclude the argument, we need again to distinguish the two cases $X = H_{\#}^1(\Omega)$ and $X = H_0^1(\Omega)$. In the former case, we can use (3.5), (3.8), (3.13) and (3.15) to get

$$\begin{aligned} \gamma \|z_v - u\|_{H^1}^2 &\leq C \left(1 + \|v\|_{L^6}^{2q} \right) \left(\|z_v - u\|_{L^2}^2 + \|z_v - u\|_{L^6} \right) \|u - v\|_{L^{\max(r, 2)}} \\ &\quad + C \|u - v\|_{L^2} \|z_v - u\|_{L^3} \|z_v - u\|_{L^6} \\ &\leq C \left(1 + \|v\|_{L^6}^{2q} \right) \|z_v - u\|_{H^1} \|u - v\|_{L^{\max(r, 2)}}, \end{aligned} \quad (3.31)$$

where we have used that $\|z_v - u\|_{L^2} \leq \|z_v\|_{L^2} + \|u\|_{L^2} = 2$. In the latter case, from (3.5), (3.9) and (3.16) we have

$$\begin{aligned} \gamma \|z_v - u\|_{H^1}^2 &\leq \frac{1}{2} \left(2\varepsilon + C_{\varepsilon} \left(1 + \|v\|_{L^6}^{2q} \right) \|u - v\|_{L^{\max(r, 2)}} \right) \|z_v - u\|_{L^2}^2 \\ &\quad + C \left(1 + \|v\|_{L^6}^{2q} \right) \|z_v - u\|_{L^6} \|u - v\|_{L^r} \\ &\quad + \varepsilon \|z_v - u\|_{L^2}^2 + C_{\varepsilon} \|u - v\|_{L^2} \|z_v - u\|_{L^3} \|z_v - u\|_{L^6}. \end{aligned} \quad (3.32)$$

We can choose $\varepsilon = \gamma/4$ and get (3.14). This completes the proof. \square

Proof of Lemma 3.5. We first notice that if $\lambda_{2,v} \geq \lambda_{2,u}$, then

$$\lambda_{2,v} - \lambda_v \geq g + \lambda - \lambda_v,$$

so that $\lambda_{2,v} - \lambda_v \geq g/2$ follows from (3.15) and (3.16) provided $\|u - v\|_{H^1}$ being small enough.

Let us now deal with the case where $\lambda_{2,v} < \lambda_{2,u}$. Since

$$\lambda_{2,u} = \langle A_u z_{2,u}, z_{2,u} \rangle \leq C,$$

we have

$$\forall v \in X, \quad \lambda_{2,v} < C.$$

On the other hand, using again (3.3), we get

$$\forall v \in X, \quad \lambda_{2,v} = \langle A_v z_{2,v}, z_{2,v} \rangle \geq \frac{\alpha}{2} \|z_{2,v}\|_{H^1}^2 - \frac{\alpha}{2} - \beta_0.$$

Hence, there exists a constant $C \in \mathbb{R}_+$ such that

$$\forall v \in X, \quad \|z_{2,v}\|_{H^1} \leq C. \quad (3.33)$$

We now decompose $z_{2,v}$ as $z_{2,v} = (u, z_{2,v})_{L^2} u + \alpha_{2,v} z_{2,v}^\perp$ with $\alpha_{2,v} \geq 0$ and $z_{2,v}^\perp \in u^\perp$ such that $\|z_{2,v}^\perp\|_{L^2} = 1$. We have

$$\alpha_{2,v}^2 = 1 - (u, z_{2,v})_{L^2}^2 = 1 - (u - z_v, z_{2,v})_{L^2}^2 \geq 1 - \|u - z_v\|_{L^2}^2. \quad (3.34)$$

We deduce from (3.14) that there exists $0 < \eta_0 \leq 1$ such that

$$\forall v \in \mathcal{B}_{u, \eta_0}, \quad \|u - z_v\|_{H^1} \leq 1/2,$$

where \mathcal{B}_{u, η_0} is the ball in H^1 with center u and radius η_0 . It then follows from (3.34) that

$$\forall v \in \mathcal{B}_{u, \eta_0}, \quad \frac{1}{\alpha_{2,v}^2} \leq 1 + 2\|u - z_v\|_{L^2}^2.$$

As $\lambda_{2,u}$ is the smallest eigenvalue of A_u in u^\perp , we obtain, using again (3.34) and the above estimate,

$$\begin{aligned} \forall v \in \mathcal{B}_{u, \eta_0}, \quad \lambda_{2,u} &\leq \langle A_u z_{2,v}^\perp, z_{2,v}^\perp \rangle \\ &= \frac{1}{\alpha_{2,v}^2} \langle A_u (z_{2,v} - (u, z_{2,v})_{L^2} u), z_{2,v} - (u, z_{2,v})_{L^2} u \rangle \\ &= \frac{1}{\alpha_{2,v}^2} (\langle A_u z_{2,v}, z_{2,v} \rangle - \lambda (u, z_{2,v})_{L^2}^2) \\ &\leq \frac{1}{\alpha_{2,v}^2} (\langle A_u z_{2,v}, z_{2,v} \rangle + |\lambda| \|u - z_v\|_{L^2}^2) \\ &= \frac{1}{\alpha_{2,v}^2} \left(\langle A_v z_{2,v}, z_{2,v} \rangle + \int_{\Omega} (f(u^2) - f(v^2)) z_{2,v}^2 + |\lambda| \|u - z_v\|_{L^2}^2 \right) \\ &\leq (1 + 2\|u - z_v\|_{L^2}^2) \left(\lambda_{2,v} + |\lambda| \|u - z_v\|_{L^2}^2 + \int_{\Omega} (f(u^2) - f(v^2)) z_{2,v}^2 \right), \end{aligned}$$

hence

$$\lambda_{2,v} - \lambda_{2,u} \geq -(\lambda_v - \lambda) - 2\lambda_{2,v} \|u - z_v\|_{L^2}^2 - (1 + 2\|u - z_v\|_{L^2}^2) \left(|\lambda| \|u - z_v\|_{L^2}^2 + \int_{\Omega} (f(u^2) - f(v^2)) z_{2,v}^2 \right).$$

Therefore, for any $v \in \mathcal{B}_{u, \eta_0}$, we have

$$\begin{aligned} \lambda_{2,v} - \lambda_v &\geq g - (\lambda_v - \lambda) - 2\lambda_{2,v} \|u - z_v\|_{L^2}^2 \\ &\quad - (1 + 2\|u - z_v\|_{L^2}^2) \left(|\lambda| \|u - z_v\|_{L^2}^2 + \int_{\Omega} (f(u^2) - f(v^2)) z_{2,v}^2 \right). \end{aligned} \quad (3.35)$$

The existence of some $0 < \eta \leq \eta_0$ such that $\lambda_{2,v} - \lambda_v \geq g/2$ for all $v \in \mathcal{B}_{u, \eta}$ easily follows from (3.14), (3.15), (3.16), (3.33) and (3.35) also in the case where $\lambda_{2,v} < \lambda_{2,u}$. \square

Proof of Proposition 3.1. Let $0 < \eta \leq 1$ be as in Lemma 3.5, $v \in X$ such that $\|u - v\|_{H^1} \leq \eta$, and $w \in X$ such that $\|w\|_{L^2} = 1$ and $(w, z_v)_{L^2} \geq 0$. Note that $\|v\|_{H^1} \leq \|u\|_{H^1} + 1$. Using (3.3), (3.13) and the fact that f is non-negative on \mathbb{R}_+ , we have

$$\begin{aligned} \forall z \in X, \quad \langle (A_v - \lambda_v)z, z \rangle_{X', X} &= a(z, z) + \int_{\Omega} f(v^2) z^2 - \lambda_v \|z\|_{L^2}^2 \\ &\geq \frac{\alpha}{2} \|\nabla z\|_{L^2}^2 - (\lambda_v + \beta_0) \|z\|_{L^2}^2 \\ &\geq \frac{\alpha}{2} \|\nabla z\|_{L^2}^2 - \beta \|z\|_{L^2}^2, \end{aligned}$$

where the constant β is independent of v and z . In particular,

$$\langle (A_v - \lambda_v)(w - z_v), (w - z_v) \rangle_{X', X} \geq \frac{\alpha}{2} \|\nabla(w - z_v)\|_{L^2}^2 - \beta \|w - z_v\|_{L^2}^2. \quad (3.36)$$

From Lemma 3.5, we see that for all $z \in X$ such that $(z, z_v) \geq 0$,

$$\langle (A_v - \lambda_v)z, z \rangle_{X', X} \geq \frac{g}{2} \|z - (z_v, z)_{L^2} z_v\|_{L^2}^2 = \frac{g}{2} (\|z\|_{L^2}^2 - |(z_v, z)_{L^2}|^2).$$

Therefore, we have

$$\begin{aligned} \langle (A_v - \lambda_v)(w - z_v), (w - z_v) \rangle_{X', X} &\geq \frac{g}{2} (\|w - z_v\|_{L^2}^2 - |(z_v, w - z_v)|^2) \\ &\geq \frac{g}{2} (\|w - z_v\|_{L^2}^2 - (1 - (z_v, w))) \\ &= \frac{g}{4} \|w - z_v\|_{L^2}^2. \end{aligned} \quad (3.37)$$

Combining (3.36) and (3.37) provides the lower bound of (3.17). We get the upper bound from the following estimate

$$\begin{aligned} \langle (A_v - \lambda_v)(w - z_v), (w - z_v) \rangle_{X', X} &= a(w - z_v, w - z_v) + \int_{\Omega} f(v^2)(w - z_v)^2 - \lambda_v \int_{\Omega} (w - z_v)^2 \\ &\leq C \|w - z_v\|_{H^1}^2, \end{aligned}$$

where we have used (3.3), (3.4) and (3.13). \square

3.2 Basic error analysis of scheme 1

LEMMA 3.6 Let $u_{\delta_f}^{\delta_c}$ be a solution of (2.1). Under assumptions (1.2)-(1.6), we have

$$\lim_{0 < \delta_f \leq \delta_c \rightarrow 0} \|u - u_{\delta_f}^{\delta_c}\|_{H^1} = 0.$$

Proof. In this proof, C and C_ε are constants independent of δ_c and δ_f . We first notice that

$$\|u - u_{\delta_f}^{\delta_c}\|_{H^1} \leq \|u - u_0^{\delta_c}\|_{H^1} + \|u_0^{\delta_c} - u_{\delta_f}^{\delta_c}\|_{H^1}. \quad (3.38)$$

We know from (1.11) that $\|u_{\delta_c}\|_{H^1} \leq \|u\|_{H^1} + 1$ for all $\delta_c > 0$ small enough. Using (3.14) with $v = u_{\delta_c}$ (so that $\lambda_v = \lambda_0^{\delta_c}$ and $z_v = u_0^{\delta_c}$), we obtain

$$\|u - u_0^{\delta_c}\|_{H^1} \leq C \|u - u_{\delta_c}\|_{H^1},$$

which together with (1.11) with $\delta = \delta_c$ implies

$$\lim_{\delta_c \rightarrow 0} \|u - u_0^{\delta_c}\|_{H^1} = 0. \quad (3.39)$$

For each $\delta_f > 0$, let $\Pi_{\delta_f} : X \rightarrow X_{\delta_f}$ be the orthogonal projection on X_{δ_f} for the H^1 -scalar product: for any $w \in X$,

$$\|w - \Pi_{\delta_f} w\|_{H^1} = \min_{v_{\delta_f} \in X_{\delta_f}} \|w - v_{\delta_f}\|_{H^1}.$$

Again from (1.11), for any $\eta > 0$, there exists $\delta_c^0 > 0$ such that for all $0 < \delta_c \leq \delta_c^0$, $\|u - u_{\delta_c}\|_{H^1} \leq \eta$. Assuming that $(u_{\delta_f}^{\delta_c}, u_0^{\delta_c})_{L^2} \geq 0$, we deduce from Proposition 3.1 that for all $0 < \delta_f \leq \delta_c \leq \delta_c^0$,

$$\begin{aligned}
\|u_{\delta_f}^{\delta_c} - u_0^{\delta_c}\|_{H^1}^2 &\leq c_0^{-1} \langle (A_{u_{\delta_c}} - \lambda_0^{\delta_c})(u_{\delta_f}^{\delta_c} - u_0^{\delta_c}), (u_{\delta_f}^{\delta_c} - u_0^{\delta_c}) \rangle_{X', X} \\
&= c_0^{-1} \left(\langle A_{u_{\delta_c}} u_{\delta_f}^{\delta_c}, u_{\delta_f}^{\delta_c} \rangle_{X', X} - \langle A_{u_{\delta_c}} u_0^{\delta_c}, u_0^{\delta_c} \rangle_{X', X} \right) \\
&\leq c_0^{-1} \left\langle \left\langle A_{u_{\delta_c}} \frac{\Pi_{\delta_f} u_0^{\delta_c}}{\|\Pi_{\delta_f} u_0^{\delta_c}\|_{L^2}}, \frac{\Pi_{\delta_f} u_0^{\delta_c}}{\|\Pi_{\delta_f} u_0^{\delta_c}\|_{L^2}} \right\rangle_{X', X} - \langle A_{u_{\delta_c}} u_0^{\delta_c}, u_0^{\delta_c} \rangle_{X', X} \right\rangle \\
&= c_0^{-1} \left\langle (A_{u_{\delta_c}} - \lambda_0^{\delta_c}) \left(\frac{\Pi_{\delta_f} u_0^{\delta_c}}{\|\Pi_{\delta_f} u_0^{\delta_c}\|_{L^2}} - u_0^{\delta_c} \right), \left(\frac{\Pi_{\delta_f} u_0^{\delta_c}}{\|\Pi_{\delta_f} u_0^{\delta_c}\|_{L^2}} - u_0^{\delta_c} \right) \right\rangle_{X', X} \\
&\leq c_0^{-1} C_0 \left\| \frac{\Pi_{\delta_f} u_0^{\delta_c}}{\|\Pi_{\delta_f} u_0^{\delta_c}\|_{L^2}} - u_0^{\delta_c} \right\|_{H^1}^2 \\
&\leq c_0^{-1} C_0 \left(1 + \frac{\|\Pi_{\delta_f} u_0^{\delta_c}\|_{H^1}}{\|\Pi_{\delta_f} u_0^{\delta_c}\|_{L^2}} \right)^2 \| \Pi_{\delta_f} u_0^{\delta_c} - u_0^{\delta_c} \|_{H^1}^2 \\
&\leq c_0^{-1} C_0 \left(1 + \frac{\|u_0^{\delta_c}\|_{H^1}}{\|\Pi_{\delta_f} u_0^{\delta_c}\|_{L^2}} \right)^2 \| \Pi_{\delta_f} u_0^{\delta_c} - u_0^{\delta_c} \|_{H^1}^2.
\end{aligned}$$

Since $\lim_{\delta_f \rightarrow 0} \|u_0^{\delta_c} - \Pi_{\delta_f} u_0^{\delta_c}\|_{L^2} = 0$ and $\|u_0^{\delta_c}\|_{L^2} = 1$, there exists $\delta_f^0 > 0$ such that

$$\forall 0 < \delta_f \leq \delta_f^0, \quad \|\Pi_{\delta_f} u_0^{\delta_c}\|_{L^2} \geq \frac{1}{2}.$$

It follows that for $0 < \delta_f \leq \delta_c \leq \delta_f^0$,

$$\lim_{\delta_f \rightarrow 0} \|u_{\delta_f}^{\delta_c} - u_0^{\delta_c}\|_{H^1} = 0,$$

which, together with (3.38) and (3.39), leads to the desired result. \square

LEMMA 3.7 Let $P_{\delta_f} : u^\perp \rightarrow u^\perp \cap X_{\delta_f}$ be the projection operator defined by

$$\forall w_{\delta_f} \in u^\perp \cap X_{\delta_f}, \quad \forall v \in u^\perp, \quad (v - P_{\delta_f} v, w_{\delta_f})_{H^1} = 0.$$

We have

$$\|v - P_{\delta_f} v\|_{H^1} \leq C \min_{v_{\delta_f} \in X_{\delta_f}} \|v - v_{\delta_f}\|_{H^1}.$$

Proof. For any $v \in u^\perp$, we have

$$\left(\Pi_{\delta_f} v - \frac{(\Pi_{\delta_f} v, u)_{L^2} \Pi_{\delta_f} u}{(\Pi_{\delta_f} u, u)_{L^2}} \right) \in u^\perp \cap X_{\delta_f},$$

so that

$$\begin{aligned}
\|v - P_{\delta_f} v\|_{H^1} &\leq \left\| v - \Pi_{\delta_f} v + \frac{(\Pi_{\delta_f} v, u)_{L^2} \Pi_{\delta_f} u}{(\Pi_{\delta_f} u, u)_{L^2}} \right\|_{H^1} \\
&\leq \|v - \Pi_{\delta_f} v\|_{H^1} + \left\| \frac{(\Pi_{\delta_f} v - v, u)_{L^2} \Pi_{\delta_f} u}{(\Pi_{\delta_f} u, u)_{L^2}} \right\|_{H^1} \\
&\leq \left(1 + \frac{\|\Pi_{\delta_f} u\|_{H^1}}{(\Pi_{\delta_f} u, u)_{L^2}} \right) \|v - \Pi_{\delta_f} v\|_{H^1} \\
&\leq C \min_{v_{\delta_f} \in X_{\delta_f}} \|v_{\delta_f} - v\|_{H^1}.
\end{aligned} \tag{3.40}$$

This completes the proof. \square

In order to state the main result of this section, we need to introduce the following object: for all $v \in L^2(\Omega)$, we denote by $\psi_v \in u^\perp$ the unique solution to the adjoint problem: find $\psi_v \in u^\perp$ such that

$$\forall w \in u^\perp, \quad \langle (A_u - \lambda) \psi_v, w \rangle_{X', X} = (v, w)_{L^2}. \tag{3.41}$$

The existence and uniqueness of the solution to (3.41) is a straightforward consequence of (3.11) and Lax-Milgram lemma. It follows from (3.11) that

$$\forall v \in L^2(\Omega), \quad \|\psi_v\|_{H^1} \leq M_2^{-1} \|v\|_{X'} \leq M_2^{-1} \|v\|_{L^2}.$$

THEOREM 3.2 Under assumptions (1.2)-(1.6), there exist $\delta_1 > 0$ and $C \in \mathbb{R}_+$ such that for all $0 < \delta_f \leq \delta_c \leq \delta_1$,

$$\frac{\gamma}{2} \|u - u_{\delta_f}^{\delta_c}\|_{H^1}^2 \leq E(u_{\delta_f}^{\delta_c}) - E(u) \leq C \|u - u_{\delta_f}^{\delta_c}\|_{H^1}^2 \tag{3.42}$$

and for all r such that $\frac{6}{5} \leq r = \frac{6}{5-2q} < 6$:

$$\|u - u_{\delta_f}^{\delta_c}\|_{H^1} \leq C \left(\min_{v_{\delta_f} \in X_{\delta_f}} \|u - v_{\delta_f}\|_{H^1} + \|u - u_{\delta_c}\|_{L^r} + \|u - u_{\delta_f}^{\delta_c}\|_{L^r} \right), \tag{3.43}$$

$$|\lambda - \lambda_{\delta_f}^{\delta_c}| \leq C \left(\|u - u_{\delta_f}^{\delta_c}\|_{H^1}^2 + \|u - u_{\delta_c}\|_{L^r} + \|u - u_{\delta_f}^{\delta_c}\|_{L^r} \right), \tag{3.44}$$

$$\begin{aligned}
\|u - u_{\delta_f}^{\delta_c}\|_{L^2}^2 &= \int_{\Omega} (f(u_{\delta_c}^2) - f(u^2)) u_{\delta_f}^{\delta_c} P_{\delta_f} \psi + (\lambda - \lambda_{\delta_f}^{\delta_c}) \int_{\Omega} (u_{\delta_f}^{\delta_c} - u) P_{\delta_f} \psi \\
&\quad + \langle (A_u - \lambda)(\psi - P_{\delta_f} \psi), (u - u_{\delta_f}^{\delta_c}) \rangle_{X', X} + \frac{1}{4} \|u - u_{\delta_f}^{\delta_c}\|_{L^2}^4,
\end{aligned} \tag{3.45}$$

where we have set $\psi = \psi_{u - u_{\delta_f}^{\delta_c}}$.

Proof. Let us recall that for all $w \in X$ such that $\|w\|_{L^2} = 1$,

$$\begin{aligned}
E(w) - E(u) &= \frac{1}{2} \langle (A_u - \lambda)(w - u), (w - u) \rangle_{X', X} \\
&\quad + \frac{1}{2} \int_{\Omega} (F(w^2) - F(u^2) - f(u^2)(w^2 - u^2)).
\end{aligned} \tag{3.46}$$

This equality, referred to as (32) in Cancès *et al.* (2010), can be derived easily. Using (3.12) and the convexity of F , we obtain, for $w = u_{\delta_f}^{\delta_c}$,

$$E(u_{\delta_f}^{\delta_c}) - E(u) \geq \frac{\gamma}{2} \|u - u_{\delta_f}^{\delta_c}\|_{H^1}^2,$$

that is the lower bound in (3.42). We now observe that

$$\begin{aligned} F(w^2) - F(u^2) - f(u^2)(w^2 - u^2) &= (w^2 - u^2) \int_0^1 (f(u^2 + t(w^2 - u^2)) - f(u^2)) dt \\ &= (w^2 - u^2)^2 \int_0^1 \left(\int_0^t f'(u^2 + s(w^2 - u^2)) ds \right) dt \\ &= (w^2 - u^2)^2 \int_0^1 (1-s) f'(u^2 + s(w^2 - u^2)) ds. \end{aligned} \quad (3.47)$$

We are led to split the domain Ω into four parts

$$\Omega_1 = \{x \in \Omega, u(x) < \frac{|w(x)|}{2}\}, \quad \Omega_2 = \{x \in \Omega, \frac{|w(x)|}{2} \leq u(x) < |w(x)|\},$$

$$\Omega_3 = \{x \in \Omega, |w(x)| \leq u(x) < 2|w(x)|\} \quad \text{and} \quad \Omega_4 = \{x \in \Omega, u(x) \geq 2|w(x)|\},$$

where we remark that, over $\Omega_2 \cup \Omega_3$, $|w(x)| \leq 2\|u\|_{L^\infty}$. Hence, from the assumption (1.6) made on $F'' = f'$, we deduce that $(u^2 + s(w^2 - u^2)) (f'(u^2 + s(w^2 - u^2)))$ is bounded over $\Omega_2 \cup \Omega_3$ by a constant (say C_3).

We infer from (3.10), (3.46) and (3.47) that

$$\begin{aligned} E(w) - E(u) &\leq \frac{M_1}{2} \|w - u\|_{H^1}^2 + \frac{C_3}{2} \int_{\Omega_2 \cup \Omega_3} (w^2 - u^2)^2 \left(\int_0^1 \frac{1-s}{u^2 + s(w^2 - u^2)} ds \right) \\ &\quad + \frac{1}{2} \int_{\Omega_1 \cup \Omega_4} (w^2 - u^2) \left(\int_0^1 (f(u^2 + t(w^2 - u^2)) - f(u^2)) dt \right) \\ &\leq \frac{M_1}{2} \|w - u\|_{H^1}^2 + \frac{C_3}{2} \int_{\Omega_2} \left(u^2 - w^2 - w^2 \ln \left(\frac{u^2}{w^2} \right) \right) + \frac{C_3}{2} \int_{\Omega_3} \left(u^2 - w^2 + w^2 \ln \left(\frac{w^2}{u^2} \right) \right) \\ &\quad + \frac{1}{2} \int_{\Omega_1} (u^2 - w^2) \left(\int_0^1 (f(u^2) - f(u^2 + t(w^2 - u^2))) dt \right) \\ &\quad + \frac{1}{2} \int_{\Omega_4} (w^2 - u^2) \left(\int_0^1 (f(u^2 + t(w^2 - u^2)) - f(u^2)) dt \right). \end{aligned}$$

Using that $-\ln(1-a) \leq a + 2a^2$, for any a , $0 \leq a \leq 3/4$, we first get that, on Ω_2 ,

$$(u^2 - w^2) - w^2 \ln \left(\frac{u^2}{w^2} \right) = (u^2 - w^2) - w^2 \ln \left(1 - \frac{w^2 - u^2}{w^2} \right) \leq 2 \frac{(w^2 - u^2)^2}{w^2} \leq 8(|w| - u)^2 \leq 8(w - u)^2.$$

Then, using that $\ln(1-a) \leq -a$ and $-\ln(1-a) \leq 4a$, for any a , $0 \leq a \leq 3/4$, we get that, on Ω_3 ,

$$\begin{aligned} u^2 - w^2 + w^2 \ln \left(\frac{w^2}{u^2} \right) &= u^2 - w^2 + u^2 \ln \left(1 - \frac{u^2 - w^2}{u^2} \right) + (w^2 - u^2) \ln \left(1 - \frac{u^2 - w^2}{u^2} \right) \\ &\leq 4 \frac{(w^2 - u^2)^2}{u^2} \leq 16(|w| - u)^2 \leq 16(w - u)^2. \end{aligned}$$

Finally, the facts that f is positive, increasing, and that $0 \leq |w^2 - u^2| \leq 3(|w| - u)^2 \leq 3(w - u)^2$ on $\Omega_1 \cup \Omega_4$, we get

$$\begin{aligned} E(w) - E(u) &\leq \frac{M_1}{2} \|w - u\|_{H^1}^2 + 8C_3 \int_{\Omega_2 \cup \Omega_3} (u - w)^2 + 3 \int_{\Omega_1} f(u^2) (w - u)^2 + 3 \int_{\Omega_4} f(w^2) (w - u)^2 \\ &\leq \frac{M_1}{2} \|w - u\|_{H^1}^2 + 8C_3 \int_{\Omega_2 \cup \Omega_3} (u - w)^2 + 3 \int_{\Omega_1} f(u^2) (w - u)^2 + C \int_{\Omega_4} (1 + |w|^{2q}) (w - u)^2. \end{aligned}$$

Taking $w = u_{\delta_f}^{\delta_c}$, we obtain

$$E(u_{\delta_f}^{\delta_c}) - E(u) \leq M_2 \|u - u_{\delta_f}^{\delta_c}\|_{H^1}^2,$$

where the constant M_2 depends on the H^1 -norm of $u_{\delta_f}^{\delta_c}$, which is itself uniformly bounded when $0 < \delta_f \leq \delta_c \leq \delta_1$. The proof of (3.42) is complete.

Recall that (see (33) in Canc`es *et al.* (2010))

$$\lambda_{\delta_f}^{\delta_c} - \lambda = \langle (A_u - \lambda)(u - u_{\delta_f}^{\delta_c}), (u - u_{\delta_f}^{\delta_c}) \rangle_{X', X} + \int_{\Omega} (f(u_{\delta_c}^2) - f(u^2)) (u_{\delta_f}^{\delta_c})^2. \quad (3.48)$$

Using on the one hand (3.4) with $w = u_{\delta_f}^{\delta_c} + u_{\delta_c}$, $z = u_{\delta_f}^{\delta_c} - u_{\delta_c}$ and both $v = u$, and $v = u_{\delta_c}$, and on the other hand (3.6) with $v = u_{\delta_c}$, we get

$$\begin{aligned} \int_{\Omega} (f(u_{\delta_c}^2) - f(u^2)) (u_{\delta_f}^{\delta_c})^2 &= \int_{\Omega} (f(u_{\delta_c}^2) - f(u^2)) ((u_{\delta_f}^{\delta_c})^2 - u_{\delta_c}^2) + \int_{\Omega} (f(u_{\delta_c}^2) - f(u^2)) u_{\delta_c}^2 \\ &\leq C \left(\|u - u_{\delta_c}\|_{L^r} + \|u - u_{\delta_f}^{\delta_c}\|_{L^r} \right). \end{aligned}$$

Therefore, we obtain that for all $0 < \delta_f \leq \delta_c \leq \delta_1$,

$$|\lambda_{\delta_f}^{\delta_c} - \lambda| \leq C \left(\|u - u_{\delta_f}^{\delta_c}\|_{H^1}^2 + \|u - u_{\delta_c}\|_{L^r} + \|u - u_{\delta_f}^{\delta_c}\|_{L^r} \right). \quad (3.49)$$

Let us now estimate $\|u - u_{\delta_f}^{\delta_c}\|_{H^1}$. We have

$$\|u - u_{\delta_f}^{\delta_c}\|_{H^1} \leq \|u - u_{\delta_f}^{\delta_c*}\|_{H^1} + \|u_{\delta_f}^{\delta_c*} - u_{\delta_f}^{\delta_c}\|_{H^1}, \quad (3.50)$$

where $u_{\delta_f}^{\delta_c*}$ is defined by

$$u_{\delta_f}^{\delta_c*} = u_{\delta_f}^{\delta_c} + \left(1 - \int_{\Omega} u u_{\delta_f}^{\delta_c} \right) u. \quad (3.51)$$

It is easy to see that $v := u - u_{\delta_f}^{\delta_c*} \in u^{\perp}$ and

$$u_{\delta_f}^{\delta_c*} - u_{\delta_f}^{\delta_c} = \frac{1}{2} u \|u - u_{\delta_f}^{\delta_c}\|_{L^2}^2. \quad (3.52)$$

We then only need to estimate $\|u - u_{\delta_f}^{\delta_c*}\|_{H^1}$. With the previous notation, we have

$$\|v - \Pi_{\delta_f} v\|_{H^1} \leq \|v\|_{H^1}$$

and

$$\begin{aligned}
v - \Pi_{\delta_f} v &= u - u_{\delta_f}^{\delta_c} - u + u \int_{\Omega} uu_{\delta_f}^{\delta_c} - \Pi_{\delta_f} \left(u - u_{\delta_f}^{\delta_c} - u + u \int_{\Omega} uu_{\delta_f}^{\delta_c} \right) \\
&= -u_{\delta_f}^{\delta_c} + u \int_{\Omega} uu_{\delta_f}^{\delta_c} - \Pi_{\delta_f} \left(-u_{\delta_f}^{\delta_c} + u \int_{\Omega} uu_{\delta_f}^{\delta_c} \right) \\
&= -u_{\delta_f}^{\delta_c} + u \int_{\Omega} uu_{\delta_f}^{\delta_c} + u_{\delta_f}^{\delta_c} - \Pi_{\delta_f} u \int_{\Omega} uu_{\delta_f}^{\delta_c} \\
&= (u - \Pi_{\delta_f} u) \int_{\Omega} uu_{\delta_f}^{\delta_c}.
\end{aligned}$$

Hence,

$$\|v - \Pi_{\delta_f} v\|_{H^1} \leq c \|u - \Pi_{\delta_f} u\|_{H^1}. \quad (3.53)$$

Due to (3.11) and (3.52), we have

$$\begin{aligned}
M_2 \|v\|_{H^1}^2 &\leq \langle (A_u - \lambda)v, v \rangle_{X', X} \\
&= \langle (A_u - \lambda)(v - \Pi_{\delta_f} v), v \rangle_{X', X} + \langle (A_u - \lambda)\Pi_{\delta_f} v, u_{\delta_f}^{\delta_c} - u_{\delta_f}^{\delta_c*} \rangle_{X', X} \\
&\quad + \langle (A_u - \lambda)\Pi_{\delta_f} v, u - u_{\delta_f}^{\delta_c} \rangle_{X', X} \\
&= \langle (A_u - \lambda)(v - \Pi_{\delta_f} v), v \rangle_{X', X} - \frac{1}{2} \|u - u_{\delta_f}^{\delta_c}\|_{L^2}^2 \langle (A_u - \lambda)\Pi_{\delta_f} v, u \rangle_{X', X} \\
&\quad + \langle (A_u - \lambda)\Pi_{\delta_f} v, u - u_{\delta_f}^{\delta_c} \rangle_{X', X}.
\end{aligned} \quad (3.54)$$

For any $v_{\delta_f} \in X_{\delta_f}$, we have

$$\begin{aligned}
\langle (A_u - \lambda)(u - u_{\delta_f}^{\delta_c}), v_{\delta_f} \rangle_{X', X} &= -\langle (A_u - \lambda)u_{\delta_f}^{\delta_c}, v_{\delta_f} \rangle_{X', X} \\
&= \int_{\Omega} (f(u_{\delta_c}^2) - f(u^2)) u_{\delta_f}^{\delta_c} v_{\delta_f} - \langle (A_{u_{\delta_c}} - \lambda)u_{\delta_f}^{\delta_c}, v_{\delta_f} \rangle_{X', X} \\
&= \int_{\Omega} (f(u_{\delta_c}^2) - f(u^2)) u_{\delta_f}^{\delta_c} v_{\delta_f} + (\lambda - \lambda_{\delta_f}^{\delta_c}) \int_{\Omega} u_{\delta_f}^{\delta_c} v_{\delta_f} \\
&= \int_{\Omega} (f(u_{\delta_c}^2) - f(u^2)) (u_{\delta_f}^{\delta_c} - u) v_{\delta_f} + \int_{\Omega} (f(u_{\delta_c}^2) - f(u^2)) uv_{\delta_f} \\
&\quad + (\lambda - \lambda_{\delta_f}^{\delta_c}) \int_{\Omega} u_{\delta_f}^{\delta_c} v_{\delta_f},
\end{aligned} \quad (3.55)$$

which together with (3.4) and (3.5) implies that for any $v_{\delta_f} \in X_{\delta_f}$,

$$\langle (A_u - \lambda)(u - u_{\delta_f}^{\delta_c}), v_{\delta_f} \rangle_{X', X} \leq C(\|u - u_{\delta_f}^{\delta_c}\|_{L^r} + \|u - u_{\delta_c}\|_{L^r}) \|v_{\delta_f}\|_{H^1} + |\lambda - \lambda_{\delta_f}^{\delta_c}|. \quad (3.56)$$

From (3.54) and (3.56), we have

$$\|v\|_{H^1} \leq C \left(\|v - \Pi_{\delta_f} v\|_{H^1} + \frac{1}{2} \|u - u_{\delta_f}^{\delta_c}\|_{L^2}^2 + \|u - u_{\delta_f}^{\delta_c}\|_{L^r} + \|u - u_{\delta_c}\|_{L^r} + |\lambda - \lambda_{\delta_f}^{\delta_c}| \right). \quad (3.57)$$

Therefore, for all $0 < \delta_f \leq \delta_c \leq \delta_1$, we get from (3.49), (3.50), (3.52), (3.53) and (3.57) that

$$\|u - u_{\delta_f}^{\delta_c}\|_{H^1} \leq C(\|u - \Pi_{\delta_f} u\|_{H^1} + \|u - u_{\delta_f}^{\delta_c}\|_{L^r} + \|u - u_{\delta_c}\|_{L^r}).$$

Thus (3.43) is proved. Let us now consider the L^2 estimate and set $\psi = \psi_{u-u_{\delta_f}^{\delta_c}}$ (see (3.41)). From (3.41) and (3.52), there holds

$$\begin{aligned}
 \|u - u_{\delta_f}^{\delta_c}\|_{L^2}^2 &= \int_{\Omega} (u - u_{\delta_f}^{\delta_c})(u - u_{\delta_f}^{\delta_c*}) + \int_{\Omega} (u - u_{\delta_f}^{\delta_c})(u_{\delta_f}^{\delta_c*} - u_{\delta_f}^{\delta_c}) \\
 &= \int_{\Omega} (u - u_{\delta_f}^{\delta_c})(u - u_{\delta_f}^{\delta_c*}) + \frac{1}{2} \|u - u_{\delta_f}^{\delta_c}\|_{L^2}^2 \int_{\Omega} u(u - u_{\delta_f}^{\delta_c}) \\
 &= \int_{\Omega} (u - u_{\delta_f}^{\delta_c})(u - u_{\delta_f}^{\delta_c*}) + \frac{1}{4} \|u - u_{\delta_f}^{\delta_c}\|_{L^2}^4 \\
 &= \langle (A_u - \lambda)\psi, (u - u_{\delta_f}^{\delta_c*}) \rangle_{X',X} + \frac{1}{4} \|u - u_{\delta_f}^{\delta_c}\|_{L^2}^4.
 \end{aligned} \tag{3.58}$$

We have

$$\begin{aligned}
 \langle (A_u - \lambda)\psi, (u - u_{\delta_f}^{\delta_c*}) \rangle_{X',X} &= \langle (A_u - \lambda)\psi, (u - u_{\delta_f}^{\delta_c}) \rangle_{X',X} - \left(1 - \int_{\Omega} uu_{\delta_f}^{\delta_c}\right) \langle (A_u - \lambda)\psi, u \rangle_{X',X} \\
 &= \langle (A_u - \lambda)\psi, (u - u_{\delta_f}^{\delta_c}) \rangle_{X',X},
 \end{aligned}$$

which, together with (3.55), (3.58), and the fact that $P_{\delta_f}\psi \in u^\perp$ yields

$$\begin{aligned}
 \|u - u_{\delta_f}^{\delta_c}\|_{L^2}^2 &= \langle (A_u - \lambda)\psi, u - u_{\delta_f}^{\delta_c} \rangle_{X',X} + \frac{1}{4} \|u - u_{\delta_f}^{\delta_c}\|_{L^2}^4 \\
 &= \langle (A_u - \lambda)(u - u_{\delta_f}^{\delta_c}), P_{\delta_f}\psi \rangle_{X',X} + \langle (A_u - \lambda)(\psi - P_{\delta_f}\psi), (u - u_{\delta_f}^{\delta_c}) \rangle_{X',X} \\
 &\quad + \frac{1}{4} \|u - u_{\delta_f}^{\delta_c}\|_{L^2}^4 \\
 &= \int_{\Omega} (f(u_{\delta_c}^2) - f(u^2)) u_{\delta_f}^{\delta_c} P_{\delta_f}\psi + (\lambda - \lambda_{\delta_f}^{\delta_c}) \int_{\Omega} (u_{\delta_f}^{\delta_c} - u) P_{\delta_f}\psi \\
 &\quad + \langle (A_u - \lambda)(\psi - P_{\delta_f}\psi), (u - u_{\delta_f}^{\delta_c}) \rangle_{X',X} + \frac{1}{4} \|u - u_{\delta_f}^{\delta_c}\|_{L^2}^4,
 \end{aligned}$$

which proves (3.45). \square

4. Spectral Fourier discretization

In this section, we consider $\Omega = (0, 2\pi)^d$ with $d = 1, 2, 3$ and $X = H_{\#}^1(\Omega)$, and we make the following assumptions:

$$V \in H_{\#}^{\sigma}(\Omega) \text{ for some } \sigma > d/2, \tag{4.1}$$

$$\text{the function } F \text{ satisfies (1.4)-(1.6) and is in } C^{[\sigma]+2, \sigma-[\sigma]+\varepsilon}((0, +\infty), \mathbb{R}). \tag{4.2}$$

The positive solution u to (1.1), which satisfies the elliptic equation

$$-\Delta u + Vu + f(u^2)u = \lambda u,$$

then is in $H_{\#}^{\sigma+2}(\Omega)$ and is bounded away from 0.

A natural discretization of (1.1) consists in using a Fourier basis. Denoting for any $k \in \mathbb{Z}^d$ by $e_k(x) = (2\pi)^{-d/2} e^{ik \cdot x}$, we have for all $v \in L^2(\Omega)$,

$$v(x) = \sum_{k \in \mathbb{Z}^d} \hat{v}_k e_k(x),$$

where \hat{v}_k is the k th Fourier coefficient of v :

$$\hat{v}_k := \int_{\Omega} v(x) \overline{e_k(x)} dx = (2\pi)^{-d/2} \int_{\Omega} v(x) e^{-ik \cdot x} dx.$$

The Fourier spectral approximation of the solution to (1.1) is based on the choice

$$X_M = \left\{ \sum_{k \in \mathbb{Z}^d, |k|_* \leq M} c_k e_k, \forall k, \overline{c_k} = c_{-k} \right\},$$

where $|k|_*$ denotes either the l^2 -norm or the l^∞ -norm of the wave vector k .

Endowing $H_{\#}^{\rho}(\Omega)$ with the norm defined by

$$\|v\|_{H^{\rho}} = \left(\sum_{k \in \mathbb{Z}^d} (1 + |k|_*^2)^{\rho} |\hat{v}_k|^2 \right)^{1/2},$$

we obtain that for all $\tau \in \mathbb{R}$, and all $v \in H_{\#}^{\tau}(\Omega)$, the best approximation of v in $H_{\#}^{\rho}(\Omega)$ for any $\rho \leq \tau$ is

$$\Pi_M v = \sum_{k \in \mathbb{Z}^d, |k|_* \leq M} \hat{v}_k e_k.$$

For all real numbers ρ and τ with $\rho \leq \tau$, we have

$$\forall v \in H_{\#}^{\tau}, \quad \|v - \Pi_M v\|_{H^{\rho}} \leq \frac{1}{M^{\tau-\rho}} \|v\|_{H^{\tau}}. \quad (4.3)$$

In this section, we take $\delta_c = M^{-1}$ and $\delta_f = N^{-1}$ ($M \leq N$), and u_{δ_c} , $u_0^{\delta_c}$ and $u_{\delta_f}^{\delta_c}$ are denoted as u_M , u_0^M and u_N^M , respectively. It is easy to see that $u_0^M \in H_{\#}^{\sigma+2}(\Omega)$. Aligning the functions u_M , u_0^M and u_N^M in such a way that $(u_0^M, u_{\kappa}^M)_{L^2} \geq 0$ for $\kappa = M, N$, and using (4.3), we obtain

$$\|u_0^M - \Pi_{\kappa} u_0^M\|_{H^1} \leq \frac{1}{\kappa^{\sigma+1}} \|u_0^M\|_{H^{\sigma+2}}.$$

It therefore follows from Lemma 3.6 that

$$\lim_{0 < M \leq N \rightarrow \infty} \|u - u_N^M\|_{H^1} = 0.$$

It is proved in Cancès *et al.* (2010) that u_M converges to u in $H_{\#}^{\sigma+2}(\Omega)$. In particular, $u/2 \leq u_M \leq 2u$ on Ω for M large enough.

Besides, u_N^M is solution to the elliptic equation

$$-\Delta u_N^M + \Pi_N (V u_N^M + f(u_M^2) u_N^M) = \lambda_N^M u_N^M.$$

Thus u_N^M is uniformly bounded in $H_{\#}^2(\Omega)$, hence in $L^{\infty}(\Omega)$, and

$$\begin{aligned} \Delta(u_N^M - u) &= \Pi_N (V(u_N^M - u) + f(u_M^2) u_N^M - f(u^2) u) \\ &\quad + (\Pi_N - I)(V u + f(u^2) u) - \lambda_N^M (u_N^M - u) - (\lambda_N^M - \lambda) u. \end{aligned} \quad (4.4)$$

Since u_M is bounded in $L^\infty(\Omega)$, $F \in C^1([0, \infty), \mathbb{R}) \cap C^2((0, \infty), \mathbb{R})$, $\lim_{M \rightarrow 0} \|u - u_M\|_{H^1} = 0$, and $\lim_{0 < M \leq N \rightarrow \infty} \|u - u_N^M\|_{H^1} = 0$, the right hand side of the above equality converges to 0 in $L_\#^2(\Omega)$, which implies that $(u_N^M)_{N \in \mathbb{N}}$ actually converges to u in $H_\#^2(\Omega)$. With a bootstrapping argument, we also deduce from (4.4) that u_N^M converges to u in $H_\#^{\sigma+2}(\Omega)$.

Besides, the unique solution to (3.41) solves the elliptic equation

$$-\Delta \psi_v + (V + f(u^2) - \lambda) \psi_v = v - (v, u)_{L^2} u,$$

from which we infer that $\psi_{u-u_N^M}$ belongs to $H_\#^{\sigma+2}(\Omega)$ and $\|\psi_{u-u_N^M}\|_{H^2} \leq C \|u - u_N^M\|_{L^2}$. Hence

$$\|\psi_{u-u_N^M} - \Pi_N \psi_{u-u_N^M}\|_{H^1} \leq \frac{1}{N} \|\psi_{u-u_N^M}\|_{H^2} \leq \frac{C}{N} \|u - u_N^M\|_{L^2}.$$

THEOREM 4.1 Under assumptions (4.1)-(4.2), there exists $C \in \mathbb{R}_+$ such that for all $N \in \mathbb{N}$,

$$\|u - u_M\|_{H^\tau} \leq \frac{C}{M^{\sigma+2-\tau}} \quad \text{for all } -\sigma \leq \tau < \sigma + 2, \quad (4.5)$$

$$E(u_N^M) - E(u) \leq C \left(\frac{1}{M^{\sigma+3}} + \frac{1}{N^{\sigma+1}} \right)^2, \quad (4.6)$$

$$\|u - u_N^M\|_{H^1} \leq C \left(\frac{1}{M^{\sigma+3}} + \frac{1}{N^{\sigma+1}} \right), \quad (4.7)$$

$$\|u - u_N^M\|_{L^2} \leq C \left(\frac{1}{M^{\min\{\sigma+4, 2(\sigma+1)\}}} + \frac{1}{N} \left(\frac{1}{M^{\sigma+3}} + \frac{1}{N^{\sigma+1}} \right) \right), \quad (4.8)$$

$$|\lambda - \lambda_N^M| \leq C \left(\frac{1}{M^{2(\sigma+1)}} + \frac{1}{N^{2(\sigma+1)}} \right). \quad (4.9)$$

Proof. The proof of (4.5) is detailed in Cancès *et al.* (2010)¹.

Let us first come back to (3.48), which we rewrite as,

$$\lambda_N^M - \lambda = \langle (A_u - \lambda)(u - u_N^M), u - u_N^M \rangle_{X', X} + \int_\Omega w^{M,N}(u_M - u), \quad (4.10)$$

with

$$w^{M,N} = \frac{f(u_M^2) - f(u^2)}{u_M^2 - u^2} (u_M + u)(u_N^M)^2 = (u_M + u)(u_N^M)^2 \int_0^1 f'(u^2 + t(u_M^2 - u^2)) dt,$$

where the argument of f' , namely $(u^2 + t(u_M^2 - u^2))$, belongs to $H_\#^{\sigma+2}(\Omega)$ for any $t \in (0, 1)$. As, for M large enough, $u/2 \leq u_M \leq 2u$ on Ω for M , we also have $u^2/4 \leq (u^2 + t(u_M^2 - u^2)) \leq 4u^2$. As $f \in C^{[\sigma]+1, \sigma-[\sigma]+\varepsilon}([\|u\|_{L^\infty}^2/4, 4\|u\|_{L^\infty}^2], \mathbb{R})$, we obtain that $w^{M,N}$ is uniformly bounded in $H_\#^\sigma(\Omega)$ (at least for N large enough). We therefore infer from (4.10) that, for M large enough,

$$|\lambda_N^M - \lambda| \leq C(\|u - u_N^M\|_{H^1}^2 + \|u - u_M\|_{H^{-\sigma}}). \quad (4.11)$$

¹Note that, as already observed in Cancès *et al.* (2010), it follows from the fact that the continuous solution u and the discrete ones u_M and u_N^M are bounded away from zero, the assumption that there exist $1 < r \leq 2$ and $0 \leq s \leq 5 - r$ such that

$$\forall R > 0, \exists C_R \in \mathbb{R}_+ \text{ s.t. } \forall 0 < t_1 \leq R, \forall t_2 \in \mathbb{R}, |F'(t_2^2)t_2 - F'(t_1^2)t_2 - 2F''(t_1^2)t_1^2(t_2 - t_1)| \leq C_R(1 + |t_2|^s)|t_2 - t_1|^r$$

made in Cancès *et al.* (2010) is actually not necessary and is thus not made here.

We now make use of (3.45), which reads here as

$$\begin{aligned} \|u - u_N^M\|_{L^2}^2 &= \int_{\Omega} (f(u_M^2) - f(u^2)) u_N^M P_N \psi + (\lambda - \lambda_N^M) \int_{\Omega} (u_N^M - u) P_N \psi \\ &\quad + \langle (A_u - \lambda)(\psi - P_N \psi), (u - u_N^M) \rangle_{X', X} + \frac{1}{4} \|u - u_N^M\|_{L^2}^4, \end{aligned} \quad (4.12)$$

with $\psi = \psi_{u-u_N^M}$. Reasoning as above, we obtain that the sequence

$$\tilde{w}^{M,N} = \frac{f(u_M^2) - f(u^2)}{u_M^2 - u^2} (u_M + u) u_N^M = (u_M + u) u_N^M \int_0^1 f'(u^2 + t(u_M^2 - u^2)) dt$$

is uniformly bounded in $H_{\#}^{\sigma}(\Omega)$ (at least for M large enough). Setting $\sigma^* = \min\{\sigma, 2\}$, we have

$$\begin{aligned} \int_{\Omega} (f(u_M^2) - f(u^2)) u_N^M P_N \psi &= \int_{\Omega} \tilde{w}^{M,N} P_N \psi (u_M - u) \\ &\leq \|u - u_M\|_{H^{-\sigma^*}} \|\tilde{w}^{M,N} P_N \psi\|_{H^{\sigma^*}} \\ &\leq c' \|u - u_M\|_{H^{-\sigma^*}} \|v_N\|_{H^2}, \end{aligned}$$

which, together with (3.40), (4.3) and (4.12), implies

$$\begin{aligned} \|u - u_N^M\|_{L^2}^2 &\leq C \left(\|u - u_M\|_{H^{-\sigma^*}} \|u - u_N^M\|_{L^2} + |\lambda - \lambda_N^M| \|u - u_N^M\|_{L^2}^2 \right. \\ &\quad \left. + \frac{1}{N} \|u - u_N^M\|_{H^1} \|u - u_N^M\|_{L^2} + \frac{1}{4} \|u - u_N^M\|_{L^2}^4 \right). \end{aligned}$$

Therefore, we have

$$\|u - u_N^M\|_{L^2} \leq C \left(\frac{1}{N} \|u - u_N^M\|_{H^1} + \|u - u_M\|_{H^{-\sigma^*}} \right). \quad (4.13)$$

Let $v := u_N^{M*} - u$, with u_N^{M*} being defined as in (3.51). We deduce from (3.54) and (3.55) that

$$\begin{aligned} M_2 \|v\|_{H^1}^2 &\leq \langle (A_u - \lambda)(v - \Pi_N v), v \rangle_{X', X} - \frac{1}{2} \|u - u_N^M\|_{L^2}^2 \langle (A_u - \lambda) \Pi_N v, u \rangle_{X', X} \\ &\quad + \int_{\Omega} (f(u_M^2) - f(u^2)) u_N^M \Pi_N v + (\lambda - \lambda_N^M) \int_{\Omega} u_N^M \Pi_N v. \end{aligned} \quad (4.14)$$

We also have

$$\begin{aligned} \int_{\Omega} (f(u_M^2) - f(u^2)) u_N^M \Pi_N v &= \int_{\Omega} \tilde{w}^{M,N} \Pi_N v (u_M - u) \\ &\leq \|u - u_M\|_{H^{-1}} \|\tilde{w}^{M,N} \Pi_N v\|_{H^1} \\ &\leq C \|u - u_M\|_{H^{-1}} \|v\|_{H^1}. \end{aligned} \quad (4.15)$$

From (3.10), (4.14) and (4.15), we obtain

$$M_2 \|v\|_{H^1}^2 \leq M_1 \|v - \Pi_N v\|_{H^1} \|v\|_{H^1} + \frac{1}{2} \|u - u_N^M\|_{L^2}^2 \|v\|_{H^1} \|u\|_{H^1} + (\|u - u_M\|_{H^{-1}} + |\lambda - \lambda_N^M|) \|v\|_{H^1}.$$

Therefore,

$$\|u - u_N^M\|_{H^1} \leq C (\|u - \Pi_N u\|_{H^1} + \|u - u_M\|_{H^{-1}}),$$

which together with (4.3), (4.11) and (4.13), completes the proof of (4.6)-(4.9). \square

5. Finite-element discretization

In this section, we assume that Ω is a rectangular brick of \mathbb{R}^d with $d = 1, 2, 3$ and $X = H_0^1(\Omega)$.

By elliptic regularity, the positive solution u to (1.1), which satisfies the elliptic equation

$$-\Delta u + Vu + f(u^2)u = \lambda u,$$

is in $H^2(\Omega) \cap H_0^1(\Omega)$ whenever V is in $L^2(\Omega)$, and is in $H^3(\Omega) \cap H_0^1(\Omega)$ whenever V is in $H^1(\Omega)$ (use an extension-by-symmetry argument in order to check that there are no vertex or edge singularities, and the fact that $f'(u^2)u^2 \nabla u$ is in $L^2(\Omega)$ whenever u is in $H^2(\Omega)$).

Considering a family of quasi-uniform triangulations $(\mathcal{T}_\delta)_\delta$ of Ω , we introduce the coarse $(X_H^p)_H$ (associated to the triangulations indexed by $\delta = H$) and fine $(X_h^\ell)_h$ (associated to the triangulations indexed by $\delta = h$) finite element subspaces of $H_0^1(\Omega)$ such that :

- $X_\delta^k = \{v \in H_0^1(\Omega), \forall K_\delta \in \mathcal{T}_\delta, v|_{K_\delta} \in \mathbb{P}_k(K_\delta)\},$
- $k = p$ or ℓ ($p, \ell = 1$ or 2)
- $\delta = H$ or h , with $0 < h \ll H$,
- \mathcal{T}_h is a sub-triangulation of \mathcal{T}_H .

As usual, H (resp. h) denote the maximum of the diameters $H_K, K \in \mathcal{T}_H$ (resp. $h_{K'}, K' \in \mathcal{T}_h$).

We denote by $\mathcal{I}_{\delta,k}$ the interpolation operator on X_δ^k . The following estimates are classical (see e.g. Bernardi *et al.* (2000); Ciarlet & Lions (1991); Ern & Guermond (2004)).

LEMMA 5.1 For any integer $n, 0 \leq n \leq k+1$, and for all r and $q, 1 \leq r \leq q < +\infty$, such that $\forall K_\delta \in \mathcal{T}_\delta, W^{n,r}(K_\delta)$ is included in $C^0(K_\delta)$, there exists a positive constant c depending only on n, r and q such that, for any function v of $W^{n,r}(\Omega)$, we have :

$$\|v - \mathcal{I}_{\delta,k} v\|_{L^\infty} \leq c \delta^{n-\frac{d}{r}} |v|_{W^{n,r}}, \quad (5.1)$$

$$\|v - \mathcal{I}_{\delta,k} v\|_{W^{1,q}} \leq c \delta^{n-1-\frac{d}{r}+\frac{d}{q}} |v|_{W^{n,r}}. \quad (5.2)$$

LEMMA 5.2 There exists a positive constant c independent of δ such that, for any $v_\delta \in X_\delta^k$ we have :

$$\|v_\delta\|_{L^\infty} \leq c \zeta(\delta) \|v_\delta\|_{H^1} \quad \text{where} \quad \zeta(\delta) = \begin{cases} c \|v_\delta\|_{H^1} & \text{for } d=1, \\ c(1 + |\log \delta|) \|v_\delta\|_{H^1} & \text{for } d=2, \\ c \delta^{-\frac{1}{2}} \|v_\delta\|_{H^1} & \text{for } d=3. \end{cases}$$

Let $u_{\delta,k}$ be a solution of the minimization problem

$$\inf \left\{ E(v_{\delta,k}), v_{\delta,k} \in X_\delta^k, \int_\Omega v_{\delta,k}^2 = 1 \right\}$$

such that $(u, u_{\delta,k})_{L^2} \geq 0$. Let us recall the main result in Cancès *et al.* (2010) concerning the finite element discretization.

THEOREM 5.1 Assume that

$$V \in L^2(\Omega), \quad \text{the function } F \text{ satisfies (1.4), (1.5) for } q = 1, \text{ and (1.6),} \quad (5.3)$$

and there exist $1 < r \leq 2$ and $0 \leq s + r \leq 3$ such that $\forall R > 0, \exists C_R \in \mathbb{R}_+$ for which

$$\forall 0 < t_1 \leq R, \forall t_2 \in \mathbb{R}, |F'(t_2^2)t_2 - F'(t_1^2)t_2 - 2F''(t_1^2)t_1^2(t_2 - t_1)| \leq C_R(1 + |t_2|^s)|t_2 - t_1|^r. \quad (5.4)$$

Then there exist $\delta_0 > 0$ and $C \in \mathbb{R}_+$ such that for all $0 < \delta \leq \delta_0$, $k = 1$ or $k = 2$

$$\|u_{\delta,k} - u\|_{H^1} \leq C\delta \|u\|_{H^2}, \quad (5.5)$$

$$\|u_{\delta,k} - u\|_{L^2} \leq C\delta^2 \|u\|_{H^2}, \quad (5.6)$$

$$\|u_{\delta,k} - u\|_{H^{-1}} \leq C\delta^2 \|u\|_{H^2}, \quad (5.7)$$

$$|\lambda_{\delta,k} - \lambda| \leq C\delta^2 \|u\|_{H^2}. \quad (5.8)$$

If, in addition,

$$V \in H^1(\Omega), \text{ (5.4) is satisfied for } r = 2, F \in C^3((0, +\infty), \mathbb{R}), \quad (5.9)$$

$$F \in C^3((0, +\infty), \mathbb{R}) \text{ and } F''(t)t^{1/2} \text{ and } F'''(t)t^{3/2} \text{ are locally bounded in } [0, +\infty), \quad (5.10)$$

then there exist $\delta_0 > 0$ and $C \in \mathbb{R}_+$ such that for all $0 < \delta \leq \delta_0$,

$$\|u_{\delta,2} - u\|_{H^1} \leq C\delta^2 \|u\|_{H^3}, \quad (5.11)$$

$$\|u_{\delta,2} - u\|_{L^2} \leq C\delta^3 \|u\|_{H^3}, \quad (5.12)$$

$$\|u_{\delta,2} - u\|_{H^{-1}} \leq C\delta^4 \|u\|_{H^3}, \quad (5.13)$$

$$|\lambda_{\delta,2} - \lambda| \leq C\delta^4 \|u\|_{H^3}. \quad (5.14)$$

In this section, we will take $X_{\delta_c} = X_H^p$, and $X_{\delta_f} = X_h^\ell$. Let $u_0^{H,p} \in X$ be the unique solution of

$$J_{H,p} = \inf \left\{ E^{H,p}(v), v \in X, \int_{\Omega} v^2 = 1 \right\}, \quad \text{with} \quad E^{H,p}(v) = \frac{1}{2}a(v, v) + \frac{1}{2} \int_{\Omega} f(u_{H,p}^2)v^2,$$

and $u_{\delta_f}^{\delta_c} = u_{h,\ell}^{H,p}$ be the solution of the following lineared eigenvalue problem (Two-grid scheme 1): find $u_{h,\ell}^{H,p} \in X_h^\ell$, $\|u_{h,\ell}^{H,p}\|_{L^2} = 1$, $(u_{h,\ell}^{H,p})_{L^2} \geq 0$, and $\lambda_{h,\ell}^{H,p} \in \mathbb{R}$ such that

$$a(u_{h,\ell}^{H,p}, v_h) + \int_{\Omega} f(u_{H,p}^2)u_{h,\ell}^{H,p}v_h = \lambda_{h,\ell}^{H,p} \int_{\Omega} u_{h,\ell}^{H,p}v_h \quad \forall v_h \in X_h^\ell.$$

LEMMA 5.3 If (5.3) and (5.4) are satisfied, then

$$\lim_{H \rightarrow 0} \|u - u_{H,p}\|_{L^\infty} = 0 \quad \text{with } p = 1 \text{ or } 2.$$

Proof. To establish this result, we first remark that

$$\|u - u_{H,p}\|_{L^\infty} \leq \|u_{H,p} - I_{H,p}u\|_{L^\infty} + \|I_{H,p}u - u\|_{L^\infty}.$$

From (5.1), we have

$$\lim_{H \rightarrow 0} \|I_{H,p}u - u\|_{L^\infty} = 0.$$

Using (5.2) and Lemma 5.2, we obtain

$$\begin{aligned}\|u_{H,p} - I_{H,p}u\|_{L^\infty} &\leq c\zeta(H)\|u_{H,p} - I_{H,p}u\|_{H^1} \\ &\leq c\zeta(H)(\|u_{H,p} - u\|_{H^1} + \|u - I_{H,p}u\|_{H^1}) \\ &\leq c'\zeta(H)H^p\|u\|_{H^{p+1}},\end{aligned}$$

which implies

$$\lim_{H \rightarrow 0} \|u_{H,p} - I_{H,p}u\|_{L^\infty} = 0.$$

This completes the proof. \square

The following theorem states the behavior of the two-grid approach in the finite element context.

THEOREM 5.2 If (5.3) and (5.4) are satisfied, then there exist $c \in \mathbb{R}_+$ and $h_0 \in \mathbb{R}_+$ such that for all $0 < h, H \leq h_0$, we have :

$$E(u_{h,1}^{H,1}) - E(u) \leq c(h + H^2)^2, \quad (5.15)$$

$$\|u - u_{h,1}^{H,1}\|_{H^1} \leq c(h + H^2), \quad (5.16)$$

$$\|u - u_{h,1}^{H,1}\|_{L^2} \leq c(h^2 + H^2), \quad (5.17)$$

$$|\lambda - \lambda_{h,1}^{H,1}| \leq c(h^2 + H^2). \quad (5.18)$$

If, in addition, (5.9) and (5.10) are satisfied, then there exist $c \in \mathbb{R}_+$ and $h_0 \in \mathbb{R}_+$ such that for all $0 < h, H \leq h_0$ and $p, \ell = 1$ or 2 , we have :

$$E(u_{h,\ell}^{H,p}) - E(u) \leq c(h^\ell + H^{p+1})^2, \quad (5.19)$$

$$\|u - u_{h,\ell}^{H,p}\|_{H^1} \leq c(h^\ell + H^{p+1}), \quad (5.20)$$

$$\|u - u_{h,\ell}^{H,p}\|_{L^2} \leq c(h^{\ell+1} + H^{p+1}), \quad (5.21)$$

$$|\lambda - \lambda_{h,\ell}^{H,p}| \leq c(h^{2\ell} + H^{2p}). \quad (5.22)$$

Proof. We follow step by step the same lines as in Theorem 4.1. The analysis will be done gradually under the various regularity assumptions on F . We first start with the analysis of the eigenvalues. Proceeding as in (4.10), we get

$$\lambda_{h,\ell}^{H,p} - \lambda = \langle (A_u - \lambda)(u - u_{h,\ell}^{H,p}), u - u_{h,\ell}^{H,p} \rangle_{X',X} + \int_{\Omega} w^{H,h}(u_{H,p} - u),$$

with

$$w^{H,h} = \frac{f(u_{H,p}^2) - f(u^2)}{u_{H,p}^2 - u^2} (u_{H,p} + u)(u_{h,\ell}^{H,p})^2 = (u_{H,p} + u)(u_{h,\ell}^{H,p})^2 \int_0^1 f'(u^2 + t(u_{H,p}^2 - u^2)) dt.$$

We have already derived from this equality the generic estimate (3.44), which for $q = 1$ and $r = 2$, gives

$$|\lambda - \lambda_{h,\ell}^{H,p}| \leq C(\|u - u_{h,\ell}^{H,p}\|_{H^1}^2 + \|u - u_{H,p}\|_{L^2} + \|u - u_{h,\ell}^{H,p}\|_{L^2}). \quad (5.23)$$

If V and F satisfies the additional regularity assumptions (5.9)-(5.10), then $w^{H,h}$ belongs to $H^1(\Omega)$ and

$$|\lambda - \lambda_{h,\ell}^{H,p}| \leq C\left(\|u - u_{h,\ell}^{H,p}\|_{H^1}^2 + \|u - u_{H,p}\|_{H^{-1}}\right). \quad (5.24)$$

We refer to the proof of Theorem 3 in Cancès *et al.* (2010) for details. Next for any $v_{h,\ell} \in X_h^\ell$, there holds

$$\begin{aligned} \int_{\Omega} (f(u_{H,p}^2) - f(u^2)) u_{h,\ell}^{H,p} v_{h,\ell} &= \int_{\Omega} w^{H,p}(u_{H,p} - u) u_{h,\ell}^{H,p} v_{h,\ell} \\ &\leq C \|w^{H,p}\|_{L^6} \|u_{h,\ell}^{H,p}\|_{L^6} \|v_{h,\ell}\|_{L^6} \|u_{H,p} - u\|_{L^2} \\ &\leq C \|u_{H,p} - u\|_{L^2} \|v_{h,\ell}\|_{H^1}. \end{aligned} \quad (5.25)$$

We then infer from (3.45) and (5.25) that

$$\begin{aligned} \|u_{h,\ell}^{H,p} - u\|_{L^2}^2 &= (\lambda - \lambda_{h,\ell}^{H,p}) \int_{\Omega} (u_{h,\ell}^{H,p} - u) P_{h,\ell} \psi + \int_{\Omega} (f(u_{H,p}^2) - f(u^2)) u_{h,\ell}^{H,p} P_{h,\ell} \psi \\ &\quad + \langle (A_u - \lambda)(u - u_{h,\ell}^{H,p}), \psi - P_{h,\ell} \psi \rangle_{X', X} + \frac{1}{4} \|u - u_{h,\ell}^{H,p}\|_{L^2}^4 \\ &\leq |\lambda - \lambda_{h,\ell}^{H,p}| \|u - u_{h,\ell}^{H,p}\|_{L^2}^2 + \|u - u_{H,p}\|_{L^2} \|u - u_{h,\ell}^{H,p}\|_{L^2} \\ &\quad + h \|u - u_{h,\ell}^{H,p}\|_{H^1} \|u - u_{h,\ell}^{H,p}\|_{L^2} + \frac{1}{4} \|u - u_{h,\ell}^{H,p}\|_{L^2}^4, \end{aligned}$$

Hence

$$\|u_{h,\ell}^{H,p} - u\|_{L^2} \leq C (\|u - u_{H,p}\|_{L^2} + h \|u - u_{h,\ell}^{H,p}\|_{H^1}). \quad (5.26)$$

Inserting this result in (3.43) gives

$$\|u - u_{h,\ell}^{H,p}\|_{H^1} \leq C (\|u - \Pi_{h,\ell} u\|_{H^1} + \|u - u_{H,p}\|_{L^2}),$$

which leads to (5.16) and (5.20), and then to (5.15) and (5.19). Next, from (5.26), we further deduce (5.17) and (5.21). Finally, (5.18) and (5.22) are consequences of (5.23) and (5.24) respectively. \square

6. The effect of numerical integration

Let us now sketch the effect of a practical implementation of the method, and more precisely to the numerical integration of the nonlinear term. For simplicity, we focus on the case when $A = I$, with periodic boundary conditions and $\Omega = [0, L]^3$ ($L > 0$).

For $N_g \in \mathbb{N} \setminus \{0\}$, we perform the numerical integration on the cartesian grid $\mathcal{G}_{N_g} := \frac{L}{N_g} \mathbb{Z}^3$. We now introduce the subspace

$$W_{N_g}^{1D} = \begin{cases} \text{Span} \left\{ e^{ily} \mid l \in \frac{2\pi}{L} \mathbb{Z}, |l| \leq \frac{2\pi}{L} \left(\frac{N_g-1}{2} \right) \right\} & (N_g \text{ odd}) \\ \text{Span} \left\{ e^{ily} \mid l \in \frac{2\pi}{L} \mathbb{Z}, |l| \leq \frac{2\pi}{L} \left(\frac{N_g}{2} \right) \right\} \oplus \mathbb{C} (e^{i\pi N_g y/L} + e^{-i\pi N_g y/L}) & (N_g \text{ even}), \end{cases}$$

and $W_{N_g}^{3D} = W_{N_g}^{1D} \otimes W_{N_g}^{1D} \otimes W_{N_g}^{1D}$. It is then possible to define the interpolation projector I_{N_g} from $C_{\#}^0(\Gamma, \mathbb{C})$ onto $W_{N_g}^{3D}$ by $[I_{N_g}(\phi)](x) = \phi(x)$ for any $x \in \mathcal{G}_{N_g}$.

We now consider the following approximate problem

$$\inf \{ E_{N_g}^M(v_{N,N_g}), v_{N,N_g} \in X_N, \int_{\Omega} |v_{N,N_g}|^2 = 1 \}, \quad (6.1)$$

where

$$E_{N_g}^M(v_N) = \frac{1}{2} \int_{\Omega} |\nabla v_N|^2 + \frac{1}{2} \int_{\Omega} I_{N_g}(V) v_N^2 + \frac{1}{2} \int_{\Omega} f(u_M^2) v_N^2.$$

Let us denote by u_{N,N_g}^M a solution to (6.1) such that $(u_{N,N_g}^M, u_N^M) \geq 0$. Then u_{N,N_g}^M satisfies the following Euler-Lagrange equation:

$$\langle A_{u_M} u_{N,N_g}^M, v \rangle_{X',X} + \int_{\Omega} (I_{N_g}(V) - V) u_{N,N_g}^M v = \lambda_{N,N_g}^M \int_{\Omega} u_{N,N_g}^M v \quad \forall v \in X_N.$$

LEMMA 6.1 There exists a positive constant M_3 such that

$$\forall v \in X_N \cap (u_N^M)^{\perp}, \quad \langle (A_{u_M} - \lambda_N^M) v, v \rangle \geq M_3 \|v\|_{H^1}^2,$$

and

$$E^M(u_{N,N_g}^M) - E^M(u_N^M) \geq \frac{M_3}{2} \|u_{N,N_g}^M - u_N^M\|_{H^1}^2,$$

where

$$E^M(v) = \frac{1}{2} \int_{\Omega} |\nabla v|^2 + \frac{1}{2} \int_{\Omega} V v^2 + \frac{1}{2} \int_{\Omega} f(u_M^2) v^2.$$

Proof. It is easy to see that

$$E^M(u_{N,N_g}^M) - E^M(u_N^M) = \frac{1}{2} \langle (A_{u_M} - \lambda_N^M)(u_{N,N_g}^M - u_N^M), u_{N,N_g}^M - u_N^M \rangle_{X',X}.$$

Note that λ_N^M is the variational approximation in X_N of some eigenvalue of A_{u_M} . As $(u_M)_{M \in \mathbb{N}}$ converges to u in $L^\infty(\Omega)$, $A_{u_M} - A_u$ converges to 0 in operator norm. So the n^{th} eigenvalue of A_{u_M} converges to the n^{th} eigenvalue of A_u when N goes to infinity, the convergence being uniform in n . As the sequence $(\lambda_N^M)_{N \in \mathbb{N}}$ converges to λ , the non-degenerate ground state eigenvalue of A_u , we obtain that for N large enough, λ_N^M is the non-degenerate ground state eigenvalue of A_{u_M} in X_N . We conclude the proof by proceeding as in Lemma 3.1. \square

Following step by step the same lines as in Canc`es *et al.* (2010), we can prove the following result (we omit the details here for the sake brevity).

THEOREM 6.1 Assume that $V \in H_{\#}^{\sigma}(\Omega)$ for some $\sigma > d/2$ and that the function F satisfies (1.4)-(1.6) and is in $C^{[\sigma]+2, \sigma-[\sigma]+\varepsilon}((0, +\infty), \mathbb{R})$. Then there exists $C > 0$ such that for all $N \in \mathbb{N}$,

$$E(u_{N,N_g}^M) - E(u) \leq C \left(\frac{1}{M^{\sigma+3}} + \frac{1}{N^{\sigma+1}} + \frac{N^{3/2}}{N_g^{\sigma}} \right)^2,$$

$$\|u_{N,N_g}^M - u\|_{H^1} \leq C \left(\frac{1}{M^{\sigma+3}} + \frac{1}{N^{\sigma+1}} + \frac{N^{3/2}}{N_g^{\sigma}} \right),$$

$$\|u_{N,N_g}^M - u\|_{L^2} \leq C \left(\frac{1}{M^{\sigma+3}} + \frac{1}{N^{\sigma+2}} + \frac{N^{3/2}}{N_g^{\sigma}} \right),$$

$$|\lambda_{N,N_g}^M - \lambda| \leq C \left(\frac{1}{M^{2(\sigma+1)}} + \frac{1}{N^{2(\sigma+1)}} + \frac{N^{3/2}}{N_g^{\sigma}} \right).$$

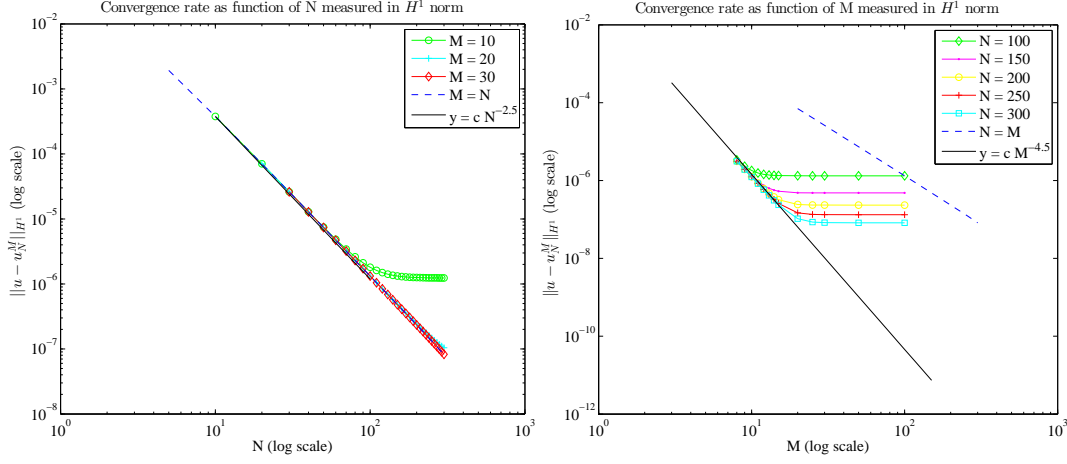


FIG. 1. Numerical errors $\|u - u_N^M\|_{H^1}$ (Fourier approximation), as functions of N (left) and M (right) (in log-log scale).

7. Numerical examples

In order to evaluate the quality of the error bounds obtained in Theorem 4.1, we have performed numerical tests with $\Omega = (0, 2\pi)$ and $f(t) = t$. The Fourier coefficients of the potential V are given by

$$\hat{V}_k = \frac{(-1)^{k+1}}{\sqrt{2\pi}} \frac{1}{|k|^2 - \frac{1}{4}},$$

from which we deduce that $V \in H_{\#}^{\sigma}(0, 2\pi)$ for all $\sigma < 3/2$. The reference values for u and λ are obtained for $N = 500$. We first fix M and study the behaviors of the numerical errors $\|u - u_N^M\|_{H^1}$, $\|u - u_N^M\|_{L^2}$, $|\lambda - \lambda_N^M|$ and $|\lambda - \tilde{\lambda}_N^M|$ as functions of N .

Let us consider for example the case when $M = 10$. From the left figures of Fig. 1 and Fig. 2 we can see that $\|u - u_N^M\|_{H^1}$ and $\|u - u_N^M\|_{L^2}$ decay respectively as $N^{-2.5}$ and $N^{-3.5}$ up to $N = 40$, while from $N = 40$ the errors decay slowly and finally reach plateaus, on which the terms in $\frac{1}{M^{\tau}}$ dominate.

Then, we fix N and study the numerical errors $\|u - u_N^M\|_{H^1}$, $\|u - u_N^M\|_{L^2}$, $|\lambda - \lambda_N^M|$ and $|\lambda - \tilde{\lambda}_N^M|$ as functions of M . From the right figures of Fig. 1 and Fig. 2 we can see that $\|u - u_N^M\|_{H^1}$ and $\|u - u_N^M\|_{L^2}$ decay respectively as $M^{-4.5}$ and M^{-5} before reaching plateaus. These results are in agreement with the assertions of Theorem 4.1.

The same conclusion holds for the error on the eigenvalue, both as a function of N or M . An interesting observation is that the two-grid scheme 1 actually leads to two approximations of the eigenvalue, the first one being $\lambda_{\delta_{\epsilon}}^{\delta_{\epsilon}}$, the second being the Rayleigh quotient (2.2). Our simulations (and this can easily be confirmed by theoretical arguments) show that the rates of convergence of these two approximations are the same. Note, however, that the accuracy is somehow better for the second approximation and that, in addition, the convergence to zero is more monotonic and smoother. We are unfortunately not able to provide an explanation of this fact.

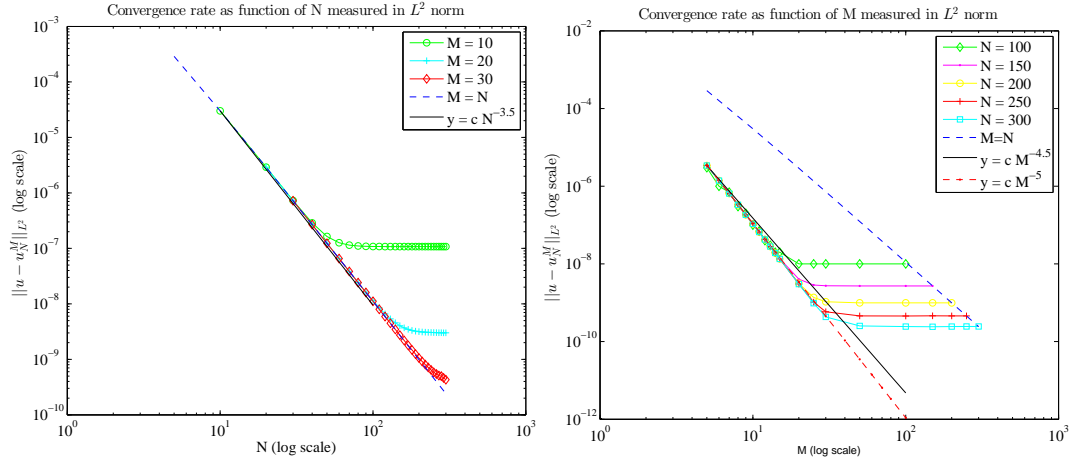


FIG. 2. Numerical errors $\|u - u_N^M\|_{L^2}$ (Fourier approximation), as functions of N (left) and M (right) (in log-log scale).

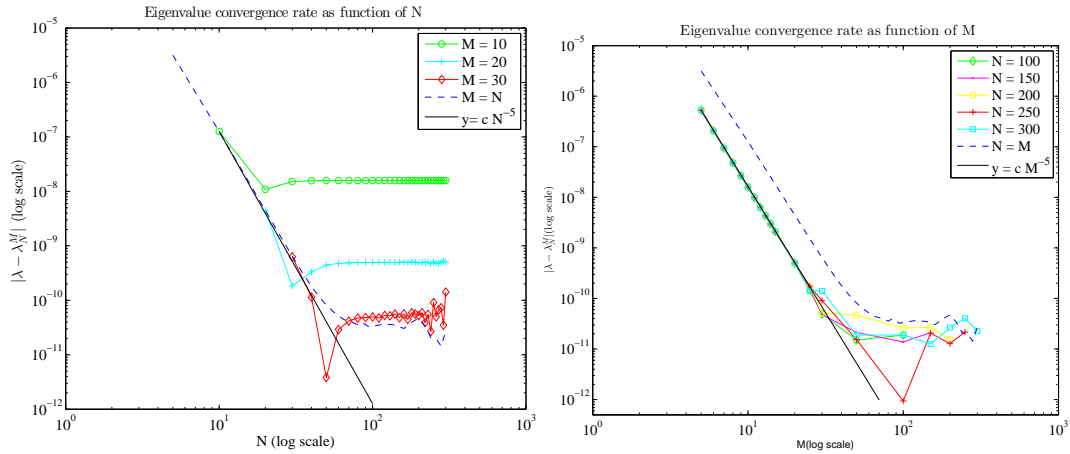


FIG. 3. Numerical errors $|\lambda - \lambda_N^M|$ (Fourier approximation), as functions of N (left) and M (right) (in log-log scale).

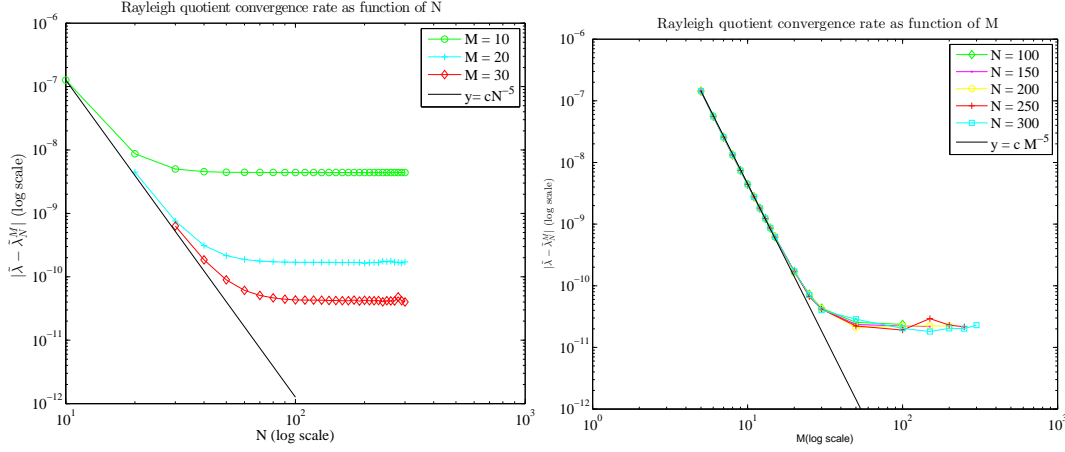


FIG. 4. Numerical errors $|\lambda - \tilde{\lambda}_N^M|$ (Fourier approximation), as functions of N (left) and M (right) (in log-log scale).

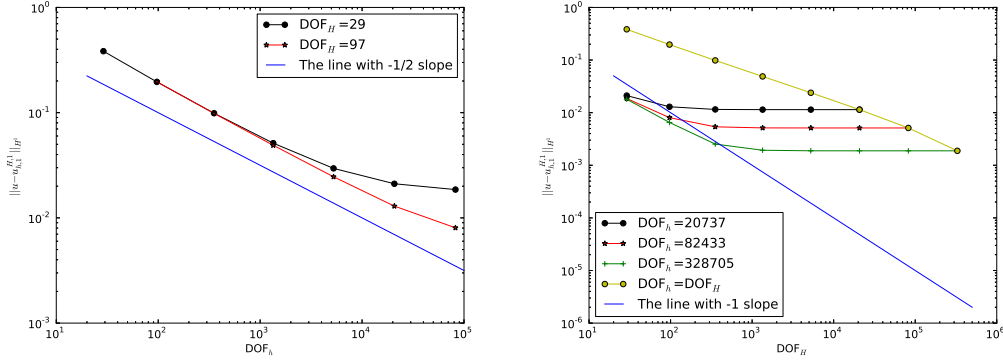
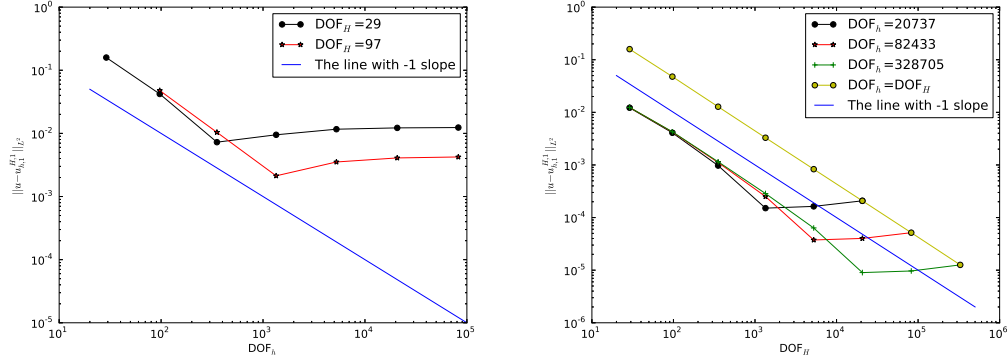
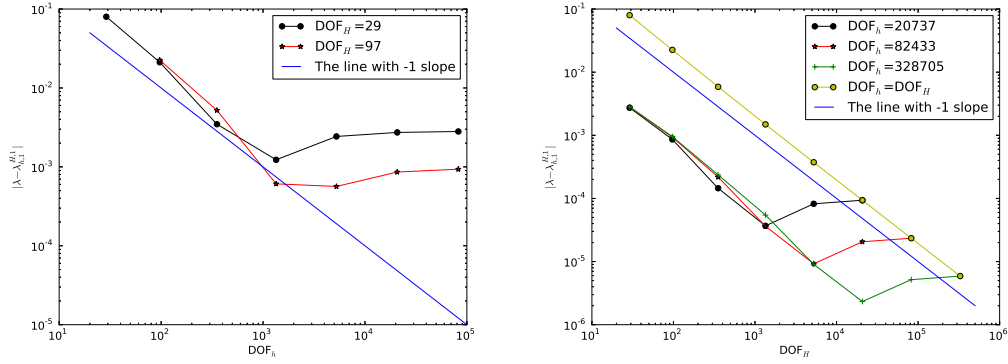
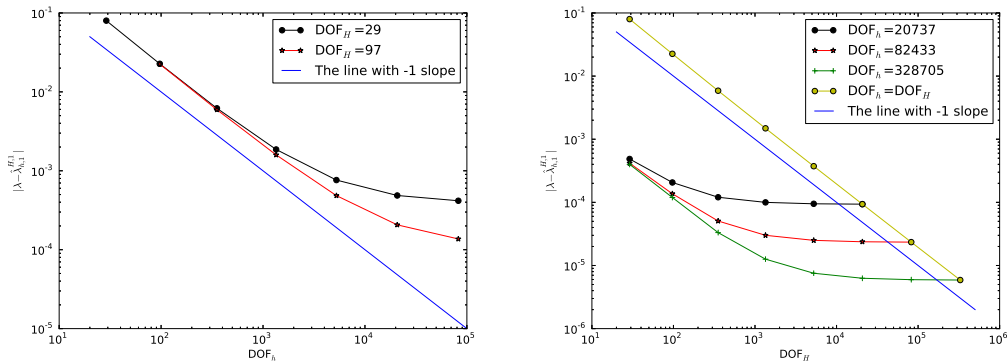


FIG. 5. Numerical errors $\|u - u_{h,1}^{H,1}\|_{H^1}$ (\mathbb{P}_1 finite elements), as functions of DOF_h (left) and DOF_H (right) (in log-log scale).

In order to evaluate the quality of the error bounds obtained in Theorem 5.2, we have performed numerical tests with $\Omega = [0, 2\pi]^2$, $f(t) = t$, $V(x) = x^2 + y^2$, using \mathbb{P}_1 and \mathbb{P}_2 finite elements. We denote the number of degrees of freedom in the coarse and fine grids by DOF_H and DOF_h , respectively.

Fig. 5-8 show the numerical errors using \mathbb{P}_1 finite elements for both the coarse grid and the fine grid. These figures agree with the results of Theorem 5.2, except the right figure of Fig. 5 in which the term in h dominates. Fig. 9-10 show the numerical errors using \mathbb{P}_1 on the coarse grid and \mathbb{P}_2 on the fine grid. Fig. 11-14 show the numerical errors using \mathbb{P}_2 finite elements on both the coarse grid and the fine grid. Similar conclusions as for the plane wave approximation hold here which illustrate the various behaviors stated in Section 5.

FIG. 6. Numerical errors $\|u - u_{h,1}^{H,1}\|_{L^2}$ (\mathbb{P}_1 finite elements), as functions of DOF_h (left) and DOF_H (right) (in log-log scale).FIG. 7. Numerical errors $|\lambda - \lambda_{h,1}^{H,1}|$ (\mathbb{P}_1 finite elements), as functions of DOF_h (left) and DOF_H (right) (in log-log scale).FIG. 8. Numerical errors $|\lambda - \tilde{\lambda}_{h,1}^{H,1}|$ (\mathbb{P}_1 finite elements), as functions of DOF_h (left) and DOF_H (right) (in log-log scale).

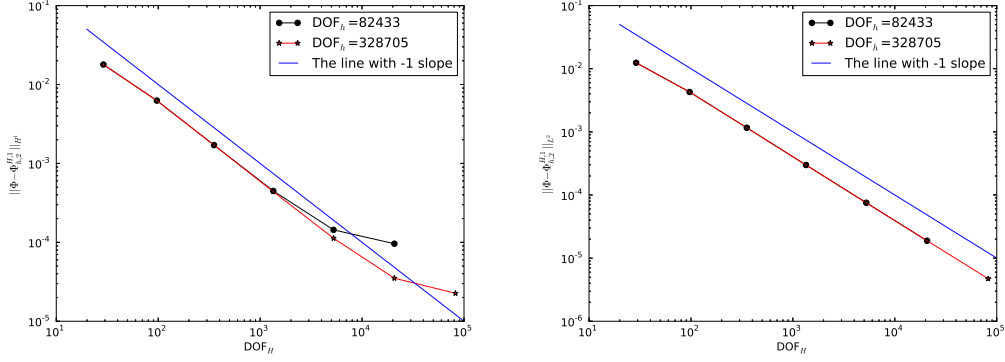


FIG. 9. Numerical errors $\|u - u_{h,2}^{H,1}\|_{H^1}$ (left) and $\|u - u_{h,2}^{H,1}\|_{L^2}$ (right), as functions of DOF_H (in log-log scale).

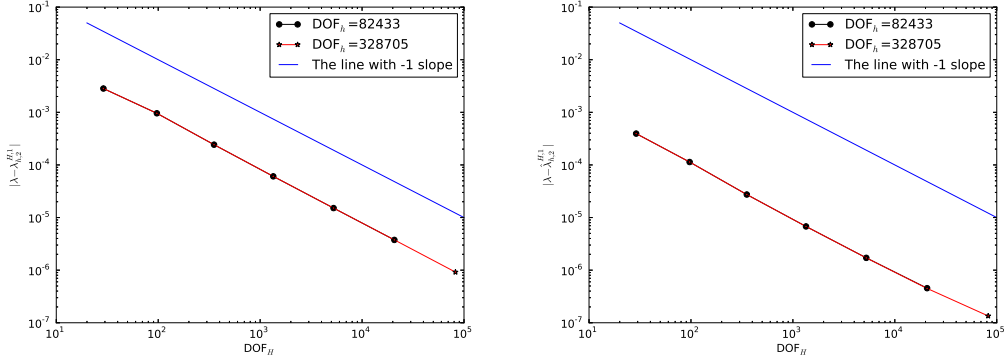
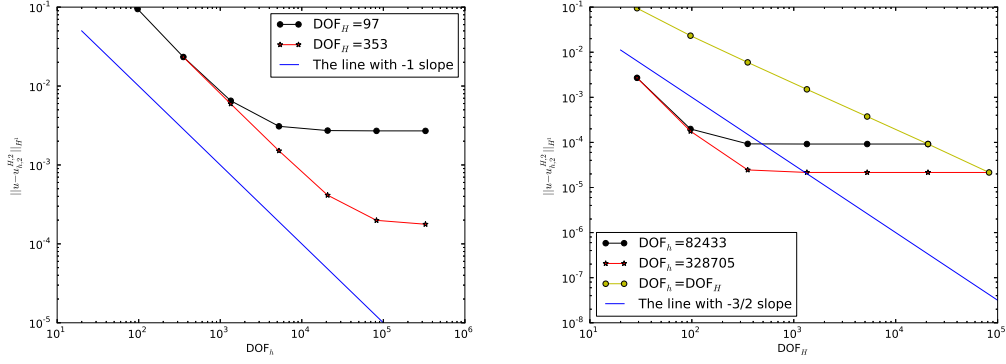
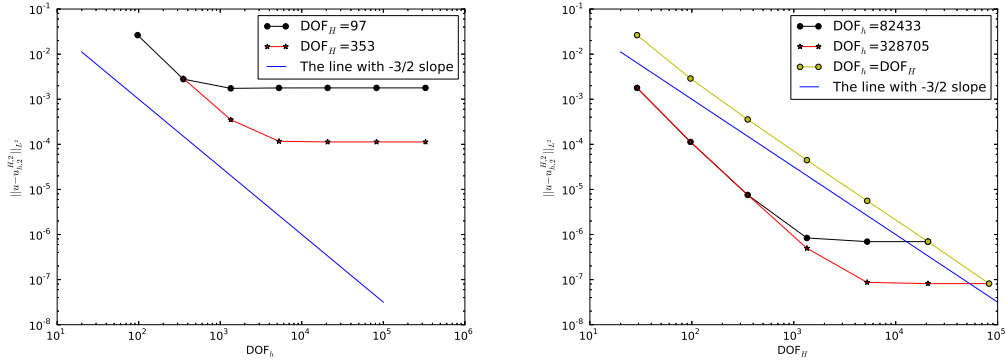
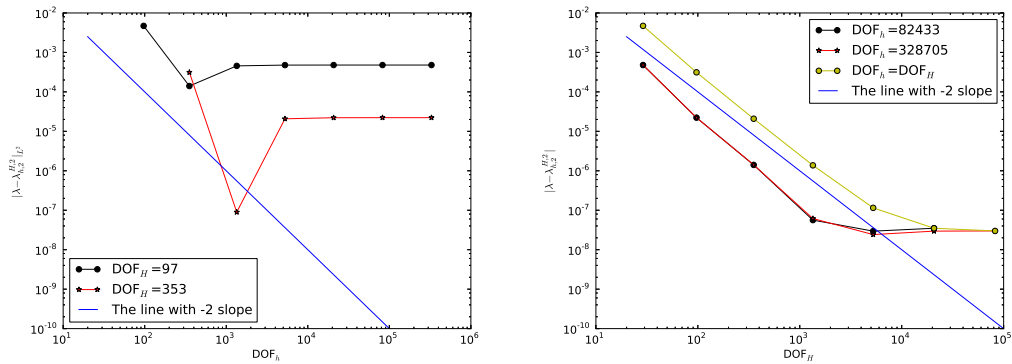


FIG. 10. Numerical errors $|\lambda - \lambda_{h,2}^{H,1}|$ (left) and $|\lambda - \tilde{\lambda}_{h,2}^{H,1}|$ (right), as functions of DOF_H (in log-log scale).

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REFERENCES

FIG. 11. Numerical errors $\|u - u_{h,2}^{H,2}\|_{H^1}$ (\mathbb{P}_2 finite elements), as functions of DOF_h (left) and DOF_H (right) (in log-log scale).FIG. 12. Numerical errors $\|u - u_{h,2}^{H,2}\|_{L^2}$ (\mathbb{P}_2 finite elements), as functions of DOF_h (left) and DOF_H (right) (in log-log scale).FIG. 13. Numerical errors $|\lambda - \lambda_{h,2}^{H,2}|$ (\mathbb{P}_2 finite elements), as functions of DOF_h (left) and DOF_H (right) (in log-log scale).

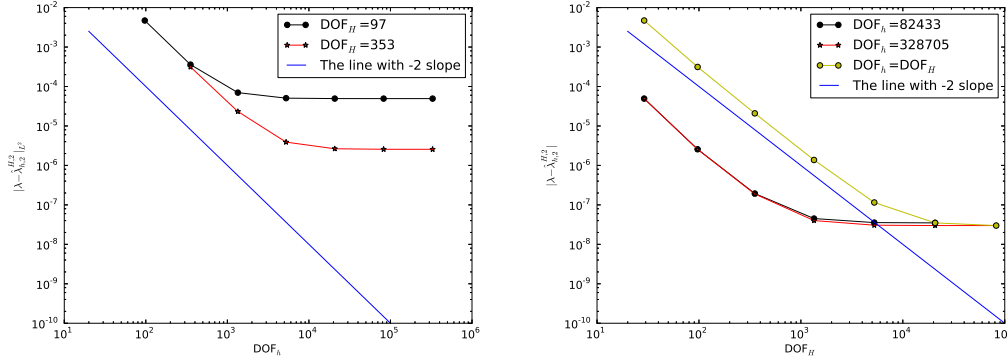


FIG. 14. Numerical errors $|\lambda - \tilde{\lambda}_{h,2}^{H,2}|$ (\mathbb{P}_2 finite elements), as functions of DOF_h (left) and DOF_H (right) (in log-log scale).

- BAO, G. & ZHOU, A. (2004) Analysis of finite dimensional approximations to a class of partial differential equations. *Math. Methods Appl. Sci.*, **27**, 2055–2066.
- BERNARDI, C., MADAY, Y. & RAPETTI, F. (2000) *Discrétisations variationnelles de problèmes aux limites elliptiques*. Springer.
- BURKE, K. (2012) Perspective on density functional theory. *J. Chem. Phys.*, **136**, 150901–150909.
- CANCÈS E., CHAKIR, R. & MADAY, Y. (2010) Numerical analysis of nonlinear eigenvalue problems. *J. Sci. Comput.*, **45**, 90–117.
- CANCÈS E., CHAKIR, R. & MADAY, Y. (2012) Numerical analysis of the plane wave discretization of some orbital-free and Kohn-Sham models. *Math. Model. Numer. Anal.*, **46**, 341–388.
- CHAKIR, R. (2009) *Contribution à l'analyse numérique de quelques problèmes en chimie quantique et mécanique*. PhD thesis, Université Pierre et Marie Curie.
- CHEN, H., GONG, X., HE, L., YANG, Z. & ZHOU, A. (2013) Numerical analysis of finite dimensional approximations of Kohn-Sham models. *Adv. Comput. Math.*, **38**, 225–256.
- CIARLET, P.G. & LIONS, J.-L. (1991) *Handbook of numerical analysis, Vol.II: Finite element methods (Part I)*. North-Holland.
- ERN, A. & GUERMOND J.-L. (2004) *Theory and practice of finite elements*. Springer.
- HENNING, P., MÅLQVIST, A. & PETERSEIM, D. (2013) Two-Level discretization techniques for ground state computations of Bose-Einstein condensates. arXiv:1305.4080
- KOHN, W. (1999) Electronic structure of matter-wave functions and density functionals. Nobel Lecture.
- KOHN, W. & SHAM, L.J. (1965) Self-consistent equations including exchange and correlation effects. *Phys. Rev.*, **140**, A1133–A1138.
- LANGWALLNER, B., ORTNER, C. & SÜLI, E. (2010) Existence and convergence results for the Galerkin approximation of an electronic density functional. *Math. Mod. Meth. Appl. Sci.*, **20**, 2237–2265.
- PERDEW, J.P. & ZUNGER, A. (1981) Self-interaction correction to density-functional approximations for many-electron systems. *Phys. Rev. B*, **23**, 5048–5079.
- PITAEVSKII, L.P. & STRINGARI, S. (2003) *Bose-Einstein Condensation*. Clarendon, Oxford.
- SICKEL, W. (1992) Superposition of functions in Sobolev spaces of fractional order. A survey. *Banach Center Publ.*, **27**, 481–497.
- XU, J. & ZHOU, A. (2000) Local and parallel finite element algorithms based on two-grid discretizations. *Math. Comput.*, **69**, 881909.

ZHOU, A. (2004) An analysis of finite-dimensional approximations for the ground state solution of Bose-Einstein condensates. *Nonlinearity*, **17**, 541–550.